```
C:\Program Files\Stnexp\Queries\10671070 (Q=N).st
                                                           [CH<sub>2</sub>]
                                                                                                                                                 -{10<del>}....</del>14 *
                                                                                                                                                      --{is}---10<sub>0</sub>10
                                                                                                 115
```

```
chain nodes :
   13 · 14 15
                   17
                            103 105
               16
                        18
ring nodes :
                                                                   35
                                                                                    39
                                                                                        40
      2 3
                5
                   6
                     7
                         8
                            9
                               10
                                  11
                                       12
                                           29
                                               30 31 32
                                                           33
                                                               34
                                                                       36
                                                                           37
                                                                               38
                                                                                            41
                                                           56 57
                                                                   58 59
                               49
                                   50 51 52
                                                   54
                                                       55
                                                                            60
                                                                               61
                                                                                   62
                                                                                        63
                                                                                            64
    42
       43
           44
                45
                   46
                        47
                            48
                                               53
                                       74
                                            75
                                                        78
                                                            79 80
                                   73
                                                76<sup>°</sup> 77
                                                                    81
                                                                       82
                                                                           88
                                                                                89
                                                                                    90
       66
           67
               68
                   69
                        70
                                72
    65
                            71
      94
    93
           95
               96
                   9,7
                        98
                            99
chain bonds :
   5-35 8-105
                       13-17 15-16 15-18 29-45 51-53 63-65 71-81
                                                                        93-95
                                                                                103-105
               13-14
ring bonds :
                        4-5 5-6 7-8
                                       7-12 8-9 9-10 10-11 11-12 29-30 29-34 30-31
    1-2 1-6
              2-3
                  3-4
                                                                                 42-43
    31-32
          32-33
                 33-34
                        35-36
                               35-40
                                       36-37
                                              37-38
                                                     38-39
                                                            39-40
                                                                   41-42
                                                                          41-46
                                                                                  55-56
    44-45
          45-46
                  47-48
                         47-52
                                48-49
                                       49-50
                                              50-51
                                                     51-52
                                                            53-54
                                                                   53-58
                                                                          54-55
                                                                                        56-57
                                                                                        69-70
    57-58
          59-60
                  59-64
                         60-61
                                61-62
                                       62-63
                                              63-64
                                                     65-66
                                                            65-70
                                                                   66-67
                                                                          67-68
                                                                                 68-69
                 72-73
                                74-75
                                       75-76
                                              77-78
                                                     77-82
                                                            78-79
                                                                   79-80
                                                                                        88-89
    71-72
          71-76
                         73-74
                                                                          80-81
                                                                                  81-82
   88-93
          89-90 90-91
                        91-92
                                92-93
                                       94-95
                                              94-99
                                                     95-96
                                                            96-97
                                                                   97-98
                                                                          98-99
exact/norm bonds :
   8-105 103-105
exact bonds :
   5-35 13-14
                13-17
                       15-16 15-18 29-45 51-53 63-65 71-81 93-95
normalized bonds :
                        4-5 5-6 7-8
                                       7-12 8-9 9-10 10-11 11-12 29-30
    1-2 1-6 2-3
                  3-4
                                                                             29-34 30-31
    31-32
          32-33
                 33-34
                        35-36
                               35-40
                                       36-37
                                              37-38
                                                     38-39 39-40
                                                                   41-42
                                                                          41-46
                                                                                 42-43
          45-46
                  47-48
                         47-52
                                48-49
                                       49-50
                                              50-51
                                                     51-52
                                                            53-54
                                                                   53-58
                                                                          54-55
                                                                                 55-56
                                                                                        56-57
    57-58
          59-60
                  59-64
                         60-61
                                61-62
                                       62-63
                                              63-64
                                                     65-66
                                                            65-70
                                                                   66-67
                                                                          67-68
                                                                                 68-69
                                                                                         69-70
    71-72
          71-76
                  72-73
                         73-74
                                74-75
                                       75-76
                                              77-78
                                                     77-82
                                                            78-79
                                                                   79-80
                                                                          80-81
                                                                                  81-82
                                                                                        88-89
    88-93 89-90
                 90-91
                        91-92
                                92-93
                                       94-95
                                             94-99
                                                     95-96
                                                            96-97
                                                                   97-98
                                                                          98-99
isolated ring systems :
```

containing 1 : 29 : 35 : 41 : 47 : 53 : 59 : 65 : 71 : 77 :

```
Match level :
```

....

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom 75:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 88:Atom 99:Atom 90:Atom 91:Atom 92:Atom 93:Atom 94:Atom 95:Atom 96:Atom 97:Atom 98:Atom 99:Atom 103:CLASS 105:CLASS

10/671,070 NCH2hand Q= RA-CH2hN. =>

Uploading C:\Program Files\Stnexp\Queries\10671070.str
*\G1^-\ch2^10CH2^3

*21-16-17²

€H2 CH2 0549

49-18-224

```
chain nodes :
13 14 16 17 18 19 21 22
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
chain bonds :
5-13 8-14 13-14 16-17 16-21 18-19 18-22
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
exact/norm bonds :
5-13 8-14 13-14 16-21 18-22
exact bonds :
16-17 18-19
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
containing 1:
```

G1:0,S,N

G2:0,S,N,[*1-*2],[*3-*4]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS Generic attributes:
13:

Saturation : Unsaturated Number of Carbon Atoms : less than 7 Number of Hetero Atoms : 2 or more Type of Ring System : Monocyclic

Element Count : Node 13: Limited

C,C4 N,N2 0,00 S, S0

L1STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

1 ANSWERS

Structure attributes must be viewed using STN Express guery preparation.

=> s 11 sss sam SAMPLE SEARCH INITIATED 13:09:29 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 584509 TO ITERATE

0.3% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **INCOMPLETE**

11647524 TO 11732836 PROJECTED ITERATIONS:

PROJECTED ANSWERS: 4820 TO 6870

L2 1 SEA SSS SAM L1

=> =>

Uploading C:\Program Files\Stnexp\Queries\10671070 (a).str

```
13 14 15 16 17 19
 ring nodes :
                       9
                         10 11
                                 12 32 33 34 35
                                                   36
                                                       37
                                                           38
 1 2 3 4 5
                   8
                          50 51 52 53 54 55 56 57 58 59 60 61 62 63
 43 44 45 46
              47
                   48
                       49
                          71 72
                                  73
                                    74
                                        75 76 77 78 79
                                                            80 81 82 83 84
 64 65 66 67
                       70
               68
                   69
                                     99
                                        100 101 104 105
 85 90 91 92 93
                       95 96 97 98
                                                            106 107 108
                   94
 110 111 112 113
                  114 115
 chain bonds :
 5-38 8-13 13-120 14-15 14-19 16-17 16-20 32-48 54-56 66-68 74-84 95-97
 109-111
 ring bonds :
-1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 32-33 32-37
                                                                44-45
 33-34 34-35 35-36 36-37 38-39
                                 38-43 39-40 40-41 41-42
                                                          42-43
             47-48 48-49 50-51
                                 50-55 51-52
                                              52-53 53-54
                                                                        56-61
 45-46 46-47
                                                           54-55
                                                                 56-57
 57-58 58-59
             59-60 60-61
                          62-63
                                 62-67 63-64
                                              64-65
                                                    65-66
                                                           66-67
                                                                 68-69
                                                                        68-73
 69-70 70-71 71-72 72-73 74-75 74-79 75-76 76-77 77-78 78-79 80-81 81-82 82-83 83-84 84-85 90-91 90-95 91-92 92-93 93-94 94-95 96-97
                                                                        96-101
 97-98 98-99 99-100 100-101 104-105 104-109 105-106 106-107 107-108
 108-109 110-111 110-115 111-112 112-113 113-114 114-115
 exact/norm bonds :
 8-13 13-120 14-19 16-20
 exact bonds :
 5-38 14-15 16-17 32-48 54-56 66-68 74-84 95-97 109-111
 normalized bonds :
 1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 32-33 32-37
 33-34 34-35 35-36 36-37 38-39 38-43 39-40 40-41 41-42 42-43 44-45 44-49
 45-46 46-47 47-48 48-49 50-51
                                50-55 51-52 52-53 53-54
                                                          54-55 56-57
 57-58 58-59 59-60 60-61 62-63
                                 62-67 63-64 64-65 65-66
                                                          66-67 68-69
 69-70 70-71
             71-72 72-73 74-75
                                 74-79 75-76 76-77 77-78 78-79 80-81 80-85
 81-82 82-83 83-84 84-85 90-91 90-95 91-92 92-93 93-94 94-95 96-97
                                                                        96-101
 97-98 98-99 99-100 100-101 104-105pad@43109 105-106 106-107 107-108
 108-109 110-111 110-115 111-112 112-113 113-114 114-115
```

chain nodes :

10/671,070 isolated ring systems : containing 1 : 32 : 38 : 44 : 50 : 56 : 62 : 68 : 74 : 80 : 90 : 96 : 104 : 110 : G1:0,S,N G2:O,S,N,[*1-*2],[*3-*4]G3: [*5], [*6], [*7], [*8], [*9], [*10], [*11] Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 19:CLASS 20:CLASS 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom 65:Atom 66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 73:Atom 74:Atom 75:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:Atom 85:Atom 90:Atom 91:Atom 92:Atom 93:Atom 94:Atom 95:Atom 96:Atom 97:Atom 98:Atom 99:Atom 100:Atom 101:Atom 104:Atom 105:Atom 106:Atom 107:Atom 108:Atom 109:Atom 110:Atom 111:Atom 112:Atom 113:Atom 114:Atom 115:Atom 120:CLASS L3 STRUCTURE UPLOADED => d 13L3 HAS NO ANSWERS L3 STR * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT * Structure attributes must be viewed using STN Express query preparation. => s 13 sss sam SAMPLE SEARCH INITIATED 13:21:16 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -7357 TO ITERATE 27.2% PROCESSED 2000 ITERATIONS 50 ANSWERS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01 FULL FILE PROJECTIONS: ONLINE **COMPLETE** BATCH **COMPLETE**

PROJECTED ITERATIONS: 141998 TO 152282 PROJECTED ANSWERS: 8457 TO 11111

L4 50 SEA SSS SAM L3

=> =>

Uploading C:\Program Files\Stnexp\Queries\10671070 (b).str

```
chain nodes :
13 14 15 16 17 19
                     20
                         106
ring nodes :
                     9
                        10
                            11
                               12 32 33 34 35 36
                                                     37
                                                         38
                                                             39
                                                                 40
                                                                        42
1 2 3 4 5
             6 7
                  8
                     49
                        50 51 52 53 54 55 56 57 58
                                                         59 60
                                                                61
                                                                     62 63
43 44 45 46 47
                  48
                         71
                             72
                                73 74 75 76 77
                                                  78
                                                     79
                                                         80
64 65 66 67
              68
                  69
                     70
                                                              81
                        97
                            98
                                99
                                   100 101 102
85 91 92 93
             94
                 95
                     96
chain bonds :
5-38 8-13 13-106 14-15 14-19 16-17 16-20 32-48 54-56 66-68
                                                              74-84
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8
                               7-12 8-9 9-10 10-11 11-12 32-33 32-37
33-34 34-35 35-36 36-37 38-39
                               38-43 39-40 40-41 41-42 42-43
                                                               44-45 44-49
45-46 46-47 47-48 48-49
                                     51-52
                                                         54-55
                        50-51
                               50-55
                                            52-53
                                                   53-54
                                                                56-57
                                                                      56-61
57-58 58-59 59-60 60-61
                               62-67 63-64
                                                                     68-73
                        62-63
                                            64-65
                                                   65-66
                                                         66-67
                                                                68-69
69-70 70-71 71-72 72-73 74-75
81-82 82-83 83-84 84-85 91-92
                               74-79 75-76
                                            76-77
                                                   77-78
                                                         78-79
                                                                     80-85
                                                               80-81
                               91-96 92-93 93-94 94-95 95-96 97-98 97-102
98-99 99-100 100-101 101-102
exact/norm bonds :
8-13 13-106 14-19 16-20
exact bonds :
5-38 14-15 16-17 32-48 54-56 66-68 74-84 96-98
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 32-33 32-37
33-34 34-35 35-36 36-37 38-39
                               38-43 39-40 40-41 41-42 42-43 44-45 44-49
                                                                     56-61
45-46 46-47 47-48 48-49 50-51
                               50-55 51-52 52-53 53-54
                                                        54-55
                                                               56-57
57-58 58-59
            59-60 60-61 62-63
                               62-67 63-64 64-65
                                                   65-66
                                                        66-67
                                                               68-69 68-73
69-70 70-71 71-72 72-73 74-75
                               74-79 75-76 76-77
                                                   77-78
                                                         78-79 80-81 80-85
81-82 82-83 83-84 84-85 91-92
                               91-96 92-93 93-94
                                                   94-95 95-96 97-98 97-102
98-99 99-100 100-101 101-102
```

isolated ring systems: containing 1: 32: 38: 44: 50: 56: 62: 68: 74: 80: G1:0,S,N G2:0,S,N,[*1-*2],[*3-*4]G3:[*5],[*6],[*7],[*8],[*9],[*10] Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 19:CLASS 20:CLASS 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom 64:Atom 65:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom 75:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 83:Atom 84:Atom 85:Atom 91:Atom 92:Atom 93:Atom 94:Atom 95:Atom 96:Atom 97:Atom 98:Atom 99:Atom 100:Atom 101:Atom 102:Atom 106:CLASS L5 STRUCTURE UPLOADED => d 15L5 HAS NO ANSWERS L5 STR * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT * Structure attributes must be viewed using STN Express query preparation. => s 15 sss sam SAMPLE SEARCH INITIATED 13:35:22 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED -7357 TO ITERATE 2000 ITERATIONS 50 ANSWERS 27.2% PROCESSED INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01 FULL FILE PROJECTIONS: ONLINE **COMPLETE** BATCH **COMPLETE** PROJECTED ITERATIONS: 141998 TO 152282 PROJECTED ANSWERS: 8115 TO 10717

L6 50 SEA SSS SAM L5

=> =>

Uploading C:\Program Files\Stnexp\Queries\10671070 (Q=N).str

```
13 14 15 16 17
                  18
                      103 105
ring nodes :
             6 7
1 2 3 4
          5
                  8
                      9
                        10
                            11
                                12
                                    29
                                       30 31 32
                                                   33
                                                      34
                                                          35
                                                              36
                         47
                            48
                                49
                                    50 51 52 53 54 55 56
                                                              57
                                                                  58
                                                                     59
                                                                         60
40 41 42 43 44
                  45
                      46
61 62
                             69
                                 70
                                     71
                                        72
                                            73
                                               74
                                                   75
                                                       76
                                                           77
                                                               78
                                                                   79
                                                                       80
                                                                          81
       63 64
              65
                  66
                      67
                         68
82 88 89 90 91
                                 96
                                     97
                                        98
                                            99
                 92
                      93
                         94
                             95
chain bonds :
5-35 8-105 13-14 13-17 15-16 15-18 29-45 51-53 63-65 71-81 93-95
                                                                      103-105
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8
                                7-12 8-9 9-10 10-11 11-12 29-30 29-34
30-31 31-32 32-33 33-34 35-36
                                35-40 36-37 37-38
                                                   38-39
                                                         39-40 41-42 41-46
42-43 43-44
            44-45
                   45-46
                         47-48
                                47-52
                                       48-49
                                             49-50
                                                    50-51
                                                          51-52
                                                                 53-54
                                                                        53-58
54-55 55-56
            56-57
                   57-58
                         59-60
                                59-64
                                      60-61
                                             61-62
                                                    62-63
                                                          63-64
                                                                 65-66
                                                                        65-70
                         71-72
                                71-76
                                      72-73
                                             73-74
                                                    74-75
                                                          75-76
                                                                 77-78
                                                                       77-82
66-67
      67-68
            68-69
                   69-70
78-79
     79-80 80-81
                   81-82
                         88-89
                                88-93 89-90
                                             90-91
                                                    91-92
                                                          92-93
                                                                 94-95
                                                                       94-99
95-96 96-97 97-98
                   98-99
exact/norm bonds :
8-105 103-105
exact bonds :
5-35 13-14 13-17 15-16 15-18 29-45 51-53 63-65 71-81 93-95
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8
                                7-12 8-9 9-10 10-11 11-12 29-30 29-34
30-31 31-32 32-33 33-34 35-36
                                35-40 36-37 37-38 38-39 39-40
                                                                41-42 41-46
            44-45 45-46 47-48
                                47-52
                                      48-49
                                             49-50
                                                   50-51
                                                          51-52
                                                                 53-54
42-43 43-44
54-55 55-56
            56-57 57-58
                         59-60
                                59-64
                                       60-61
                                             61-62
                                                    62-63
                                                          63-64
                                                                 65-66
66-67 67-68
            68-69 69-70
                         71-72
                                71-76
                                       72-73
                                             73-74
                                                   74-75
                                                          75-76
                                                                 77-78
                                                                       77-82
78-79 79-80 80-81 81-82
                         88-89
                                88-93 89-90 90-91 91-92
                                                         92-93
                                                                 94-95 94-99
95-96 96-97 97-98 98-99
```

chain nodes :

isolated ring systems: containing 1 : 29 : 35 : 41 : 47 : 53 : 59 : 65 : 71 : 77 :

G1: [*1], [*2], [*3], [*4], [*5], [*6]

G2:[*7-*8],[*9-*10]

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 57:Atom 58:Atom 59:Atom 60:Atom 61:Atom 62:Atom 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 69:Atom 70:Atom 71:Atom 72:Atom 73:Atom 74:Atom 75:Atom 76:Atom 77:Atom 78:Atom 79:Atom 80:Atom 81:Atom 82:Atom 89:Atom 90:Atom 91:Atom 92:Atom 93:Atom 94:Atom 95:Atom 96:Atom 97:Atom 98:Atom 99:Atom 103:CLASS 105:CLASS

L7 STRUCTURE UPLOADED

=> d 17

L7 HAS NO ANSWERS

L7 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s 17 sss sam
SAMPLE SEARCH INITIATED 13:40:43 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 7357 TO ITERATE

27.2% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED) SEARCH TIME: 00.00.01

23 ANSWERS

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 141998 TO 152282 PROJECTED ANSWERS: 1141 TO 2243

L8 23 SEA SSS SAM L7

=> => s 17 sss ful

FULL SEARCH INITIATED 13:44:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 147417 TO ITERATE

100.0% PROCESSED 147417 ITERATIONS 1779 ANSWERS SEARCH TIME: 00.00.02

L9 1779 SEA SSS FUL L7

=> => s 19 L10 151 L9

=> d 110 1-50 bib,ab,hitstr

```
ANSWER 1 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2006:440209 CAPLUS
DN
     144:468191
     Preparation of phenylpyrimidinecarboxamides as modulators of voltage-gated
ΤI
     sodium and calcium channels
     Martinborough, Esther; Zimmermann, Nicole; Perni, Robert; Arnost, Michael;
IN
     Bandarage, Upul; Maltais, Francois; Bemis, Guy
     Vertex Pharmaceuticals Incorporated, USA
PA
SO
     PCT Int. Appl., 166 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
                                 DATE
                                                                      DATE
     PATENT NO.
                          KIND
                                             APPLICATION NO.
                                20060511
PΙ
     WO 2006050476
                          A2
                                             WO 2005-US39881
                                                                      20051103
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
             MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
             SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
             VN, YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL,-PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, MA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ,
                                 TM
PRAI US 2004-624716P
                           P
                                 20041103
     US 2004-624718P
                                 20041103
                           Ρ
                                 20041103
     US 2004-624800P
                           Ρ
     Title compds. I [wherein \dot{X} = halo, cyano, Me, etc.; n = 1-4; R1, R2 = H,
AB
     alkyl, cycloalkyl, etc.; R3, R4 = H, alkyl, heterocyclyl, etc.; Y = H or
     alkyl] and pharmaceutically acceptable salts thereof were prepared as ion
     channel modulators, especially as voltage-gated sodium and calcium channel
     inhibitors. For instance, II was synthesized in multiple steps and showed
     inhibitory activity for CaV 2.2, Nav 1.3 and NaV 1.8 with IC50 values of <
     10.0 \mu M. I and their pharmaceutical compns. are useful for the
     treatment of various diseases.
ΙT
     886194-94-1P 886195-51-3P 886195-68-2P
     886196-06-1P 886196-52-7P 886196-53-8P
     886196-54-9P 886196-56-1P 886196-66-3P
     886196-67-4P 886196-68-5P 886196-70-9P
     886196-80-1P 886196-81-2P 886196-84-5P
     886196-87-8P 886196-90-3P 886196-92-5P
     886196-95-8P 886196-96-9P 886197-01-9P
     886197-03-1P 886197-12-2P 886197-17-7P
     886197-24-6P 886197-27-9P 886197-31-5P
     886197-33-7P 886197-36-0P 886197-37-1P
     886197-48-4P 886197-50-8P 886197-61-1P
     886197-63-3P 886197-74-6P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (inhibitor; preparation of phenylpyrimidinecarboxamides as inhibitors of
        voltage-gated sodium and calcium channels)
RN
     886194-94-1 CAPLUS
     5-Pyrimidinecarboxamide, 4-(2-fluorophenyl)-N-[(3-methoxyphenyl)methyl]-N-
CN
```

(1-methylethyl)-2-[(1-naphthalenylmethyl)amino]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A

RN 886195-51-3 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(2-fluorophenyl)-2-[[2-(4-fluorophenyl)ethyl]amino]-N-(1-methylethyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 886195-68-2 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(2-fluorophenyl)-N-(1-methylethyl)-2-[(1-naphthalenylmethyl)amino]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 886196-06-1 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(2-fluorophenyl)-N-(1-methylethyl)-N(phenylmethyl)-2-[[2-[3-(trifluoromethyl)phenyl]ethyl]amino]- (9CI) (CA
INDEX NAME)

886196-52-7 CAPLUS RN

Piperidine, 1-[[4-(4-cyanophenyl)-2-[[2-(3-fluorophenyl)ethyl]amino]-5-pyrimidinyl]carbonyl]-3,5-dimethyl- (9CI) (CA INDEX NAME) CN

RN

886196-53-8 CAPLUS Piperidine, 1-[[4-(4-cyanophenyl)-2-[[[2-(trifluoromethyl)phenyl]methyl]am CNino]-5-pyrimidinyl]carbonyl]-4-methyl- (9CI) (CA INDEX NAME)

RN 886196-54-9 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[(1,3-benzodioxol-5-ylmethyl)amino]-N-ethyl-4-(2-fluorophenyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 886196-56-1 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(2-fluorophenyl)-2-[[2-(3-fluorophenyl)ethyl]amino]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 886196-66-3 CAPLUS

CN 5-Pyrimidinecarboxamide, N-ethyl-2-[[2-(4-methoxyphenyl)ethyl]amino]-N-methyl-4-(3-methylphenyl)- (9CI) (CA INDEX NAME)

RN 886196-67-4 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[(3-chlorophenyl)methyl]amino]-N-methyl-4-(3-methylphenyl)-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

RN 886196-68-5 CAPLUS

CN Morpholine, 4-[[4-(2-fluorophenyl)-2-[[[3-(trifluoromethyl)phenyl]methyl]a mino]-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)

$$F_{3}C$$
 $CH_{2}-NH$
 N
 C
 N
 C
 N
 C

RN 886196-70-9 CAPLUS

CN Piperidine, 1-[[2-[[(3-chlorophenyl)methyl]amino]-4-(4-cyanophenyl)-5-pyrimidinyl]carbonyl]-3,5-dimethyl- (9CI) (CA INDEX NAME)

RN 886196-80-1 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(4-cyanophenyl)-N-(cyclopropylmethyl)-2-[[[2-(trifluoromethyl)phenyl]methyl]amino]- (9CI) (CA INDEX NAME)

RN 886196-81-2 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(4-cyanophenyl)-2-[[2-(3-fluorophenyl)ethyl]amino]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 886196-84-5 CAPLUS

CN Piperidine, 1-[[4-(2-fluorophenyl)-2-[[[2-(trifluoromethyl)phenyl]methyl]a mino]-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)

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RN 886196-87-8 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[(2,6-dimethoxyphenyl)methyl]amino]-4-(2-fluorophenyl)-N-methyl-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me O} \\ | & | \\ | & | \\ \text{i-Bu-N-C} \\ \hline \\ \text{F} \end{array} \qquad \begin{array}{c} \text{MeO} \\ \text{MeO} \\ \text{NH-CH}_2 \\ \\ \text{OMe} \end{array}$$

RN 886196-90-3 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[2-(4-methoxyphenyl)ethyl]amino]-N-(3-methoxypropyl)-4-(3-methylphenyl)- (9CI) (CA INDEX NAME)

RN 886196-92-5 CAPLUS

CN Pyrrolidine, 1-[[2-[(1,3-benzodioxol-5-ylmethyl)amino]-4-(4-cyanophenyl)-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)

RN 886196-95-8 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[(1,3-benzodioxol-5-ylmethyl)amino]-4-(4-cyanophenyl)-N-methyl-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

RN 886196-96-9 CAPLUS

CN Morpholine, 4-[[2-[(1,3-benzodioxol-5-ylmethyl)amino]-4-(3-methylphenyl)-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & \text{Me} \\
 & \text{O} \\
 & \text{N} \\
 & \text{O} \\
 & \text{N} \\
 & \text{NH-CH}_2
\end{array}$$

RN 886197-01-9 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[(1,3-benzodioxol-5-ylmethyl)amino]-4-(4-cyanophenyl)-N-ethyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 886197-03-1 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(4-cyanophenyl)-2-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]-N-methyl-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

RN 886197-12-2 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(4-cyanophenyl)-N-cyclohexyl-2-[[(2,6-dimethoxyphenyl)methyl]amino]-N-methyl- (9CI) (CA INDEX NAME)

RN 886197-17-7 CAPLUS

CN Piperidine, 1-[[4-(4-cyanophenyl)-2-[[2-(3,4-dimethoxyphenyl)ethyl]methyla mino]-5-pyrimidinyl]carbonyl]-3,5-dimethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} CN \\ \hline \\ N \\ \hline \\ N \\ \hline \\ N \\ \hline \\ N \\ \hline \\ CH_2 \\ \hline \\ CH_2 \\ \hline \\ OMe \\ OMe$$

RN 886197-24-6 CAPLUS

CN Pyrrolidine, 1-[[4-(4-cyanophenyl)-2-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)

RN 886197-27-9 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(4-cyanophenyl)-2-[[2-(3-fluorophenyl)ethyl]amino]-N-methyl-N-(2-methylpropyl)- (9CI) (CA INDEX NAME)

RN 886197-31-5 CAPLUS

CN 5-Pyrimidinecarboxamide, N-butyl-4-(4-cyanophenyl)-2-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]- (9CI) (CA INDEX NAME)

RN 886197-33-7 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[(1,3-benzodioxol-5-ylmethyl)amino]-4-(2-fluorophenyl)-N-(1-methylethyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 886197-36-0 CAPLUS

CN Morpholine, 4-[[4-(3-methylphenyl)-2-[(phenylmethyl)amino]-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} \\ \\ \text{Ph-CH}_2-\text{NH} \\ \\ \text{N} \\ \end{array} \begin{array}{c|c} \\ \\ \\ \\ \\ \end{array} \begin{array}{c|c} \\ \\ \\ \\ \\ \end{array} \begin{array}{c|c} \\ \\ \\ \\ \\ \end{array}$$

RN886197-37-1 CAPLUS

5-Pyrimidinecarboxamide, 2-[[2-(4-chlorophenyl)ethyl]amino]-4-(2-CN fluorophenyl)-N-(1-methylpropyl)- (9CI) (CA INDEX NAME)

RN

886197-48-4 CAPLUS
Piperidine, 1-[[4-(4-cyanophenyl)-2-[[2-(4-methoxyphenyl)ethyl]amino]-5pyrimidinyl]carbonyl]-4-methyl- (9CI) (CA INDEX NAME) CN

RN 886197-50-8 CAPLUS

CN Morpholine, 4-[[2-[[(3-chlorophenyl)methyl]amino]-4-(3-methylphenyl)-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)

RN 886197-61-1 CAPLUS

CN Piperidine, 1-[[4-(4-cyanophenyl)-2-[[2-(4-methoxyphenyl)ethyl]amino]-5-pyrimidinyl]carbonyl]-5-ethyl-2-methyl- (9CI) (CA INDEX NAME)

RN 886197-63-3 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(4-cyanophenyl)-2-[[2-(3,4-dimethoxyphenyl)ethyl]methylamino]-N-(1-methylpropyl)- (9CI) (CA INDEX NAME)

RN 886197-74-6 CAPLUS

CN Piperidine, 1-[[2-[(1,3-benzodioxol-5-ylmethyl)amino]-4-[1,1'-biphenyl]-4-yl-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)

```
ANSWER 2 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2006:411890 CAPLUS
DN
     144:450725
     Preparation of pyrazolopyrimidinones and analogs, and their compositions
ΤI
     as cannabinoid CB1 receptor inhibitors
     Liu, Hong; He, Xiaohui; Choi, Ha-Soon; Yang, Kunyong; Woodmansee, David;
IN
     Wang, Zhicheng; Ellis, David Archer; Wu, Baogen; He, Yun; Nguyen, Truc
     Ngoc
PA
     Irm LLC, Bermuda
SO
     PCT Int. Appl., 259 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
                          KIND
                                 ÐÃTE
                                             APPLICATION NO.
                                                                     DATE
     PATENT NO.
                                20060504
     WO 2006047516
                          A2
                                            WO 2005-US38361
                                                                     20051026
PΙ
         W: AE, AG, AL, AM, A\uparrow, AU, AZ, \notBA, BB, BG, BR, BW, BY, B2, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, HD, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ,
             NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG,
             SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN,
             YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NE, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ//NA, SD, SÈ, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
PRAI US 2004-622508P
                          Ρ
                                 20041026
     US 2005-672670P
                           Ρ
                                 20050418
     Title compds. I [Y = 0, NH and deri\sqrt{s}., S; R1 = (un) substituted Ph,
AB
     heteroaryl, cycloalkyl, benzyl:-R2 = (un)substituted Ph, OPh,
     heterocycloalkyl, heteroaryl; R3 = H, halo, OH, CN, etc.; R4 =
     (un) substituted hetero/aryl, alkyl, etc.; and their pharmaceutically
     acceptable salts, hydrates, solvates and isomers; with the exception of
     certain compds.] were prepared as selective cannabinoid CB1 receptor
     inhibitors. Thus, II was prepared, in 3 steps, starting from
     5-amino-1-phenyl-1H-pyrazole-4-carboxylic acid Et ester and
     2,4-dichlorobenzoyl chloride. Preferred compds. I showed a 100 fold
     selectivity for CB1 over CB2 receptor. Pharmaceutical compns. comprising
     I are useful for preventing and treating diseases or disorders associated
     with the activity of CB1 receptor, e.g. metabolic disorders.
     885619-20-5P, 5-(4-Chlorophenyl)-3-methylsulfonyl-6-[4-[2-[(4-
ΙT
     methoxybenzyl)amino]pyrimidin-4-yl]phenyl]-1-phenyl-1,5-
     dihydropyrazolo[3,4-d]pyrimidin-4-one
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (intermediate; preparation of pyrazolopyrimidinones and analogs as CB1
        inhibitors)
RN
     885619-20-5 CAPLUS
CN
     4H-Pyrazolo[3,4-d]pyrimidin-4-one, 5-(4-chlorophenyl)-1,5-dihydro-6-[4-[2-
     [[(4-methoxyphenyl)methyl]amino]-4-pyrimidinyl]phenyl]-3-(methylsulfonyl)-
     1-phenyl- (9CI) (CA INDEX NAME)
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ANSWER 3 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2006:381409 CAPLUS
DN
     144:432829
     Preparation of 2,6-substituted-4-monosubstituted amino-pyrimidines as
ΤI
     prostaglandin D2 receptor antagonists
IN
     Lim, Sungtaek; Harris, Keith John; Stefany, David; Gardner, Charles J.;
     Cao, Bin; Boffey, Ray; Gillespy, Timothy A.; Aguiar, Joacy C.; Hunt, Hazel
     J.; Dechaux, Elsa A.
     Aventis Pharmaceuticals Inc., USA
PA
SO
     PCT Int. Appl., 272 pp.
     CODEN: PIXXD2
DT
     Patent
     English
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FAN.CNT 1
                                DATE
                         KIND
                                             APPLICATION NO.
     PATENT NO.
                                                                     DATE
     WO 2006044732
                          A2
                                20060427
                                             WO 2005-US37148
                                                                     20051014
PΙ
         W: AE, AG, AL, AM, AT AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, QE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ,
             NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG,
             SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN,
             YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
PRAI US 2004-619272P
                                20041015
                          Р
     The invention is directed to the preparation of aminopyrimidines I [Cyl =
     (un) substituted cycloalkyl heterocyclyl, heterocaryl, etc.; Cy2 =
     (un) substituted cycloalkenyl, heterocyclenyl, hetero/aryl, etc.; L1 =
     cyclo/alkylene, CH2-haloalkylene; or L1Cy2 = arylcycloalkyl,
     cycloalkylaryl; R1 = alkylthio, NH2 and derivs., alkoxy; L2 = a bond, O,
     CH2O; provided that when R1 = OMe, L1 = CH2CH2, L2 = a bond, and Cy2 =
     2,4-dichlorophenyl, then Cyl is not 1-methyl-2-ethyloxycarbonylindol-5-
     yl], and their N-oxides, ester prodrugs, and their pharmaceutically
     acceptable salts, hydrates and solvates, and their use as prostaglandin D2
     (PGD2) receptor antagonists in pharmaceutical compns. comprising a
     pharmaceutically effective amount of one or more compds. I in admixt. with a
     pharmaceutically acceptable carrier, and to a method of treating a patient
     suffering from a PGD2-mediated disorder. E.g., a 4-step synthesis,
     starting from from 3-fluoro-4-methoxybenzaldehyde, was given for
     pyrimidine II. Selected I produced 50% inhibition in the SPA cAMP assay
     in human LS174T cells expressing the endogenous DP receptor at concns.
     within the range of about 0.1 to about 30 nM. I are useful for treating
     allergic disease (such as allergic rhinitis, allergic conjunctivitis,
     atopic dermatitis, bronchial asthma and food allergy), systemic
     mastocytosis, disorders accompanied by systemic mast cell activation,
     anaphylaxis shock, bronchoconstriction, bronchitis, urticaria, eczema,
     diseases accompanied by itch, diseases (such as cataract, retinal
     detachment, inflammation, infection and sleeping disorders) which are
     generated secondarily as a result of behavior accompanied by itch (such as
     scratching and beating), chronic obstructive pulmonary diseases, ischemic
     reperfusion injury, cerebrovascular accident, chronic rheumatoid
     arthritis, pleurisy, ulcerative colitis (no data).
IT
     885066-02-4P, 3-[6-[[2-(3-Fluoro-4-methoxyphenyl)ethyl]amino]-2-
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methoxypyrimidin-4-yl]benzonitrile 885066-03-5P,
[6-(3-Aminophenyl)-2-methoxypyrimidin-4-yl][2-(4-methoxyphenyl)ethyl]amine
885066-05-7P, 3-[2-Methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyri
midin-4-yl]benzenesulfonamide 885066-10-4P, [6-(3-Aminophenyl)-2-
methoxypyrimidin-4-yl][2-(4-trifluoromethoxyphenyl)ethyl]amine
885066-29-5P, 3-[2-Methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyri
midin-4-yl]benzaldehyde 885066-30-8P, [3-[6-[[2-(2-Chloro-6-
fluorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]phenyl]methanol
885066-31-9P, 3-[6-[[2-(2-Chloro-6-fluorophenyl)ethyl]amino]-2-
methoxypyrimidin-4-yl]benzaldehyde 885066-50-2P,
2-Fluoro-5-[2-methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyrimidin-4-
yl]benzaldehyde 885066-61-5P, 3-[2-Methoxy-6-[[2-(4-
methoxyphenyl)ethyl]amino]pyrimidin-4-yl]phenol 885066-63-7P,
3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]benzoic
acid 885066-65-9P, 3-[6-[[2-(2-Chloro-6-
fluorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]benzoic acid
885066-67-1P, 2-[3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-
methoxypyrimidin-4-yl]phenyl]-2-methylpropionic acid 885066-68-2P***,
[2-(3,4-Dimethoxyphenyl)ethyl][6-(3,4-dimethoxyphenyl)-2-
                                     ***885066-71-7P,
methylsulfanylpyrimidin-4-yl]amine
[2-(4-Methoxyphenyl)ethyl][6-(3-methoxyphenyl)-2-methylsulfanylpyrimidin-4-
yl]amine 885066-81-9P, 2-Methoxy-5-[2-methoxy-6-[[2-(4-
methoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzaldehyde 885066-86-4P
, 2-[3-[2-Methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyrimidin-4-
yl]phenoxy]-2-methylpropionic acid ethyl ester 885066-87-5P,
[3-[2-Methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyrimidin-4-
yl]phenoxy]acetic acid methyl ester 885066-89-7P,
3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]phenol
885066-92-2P, [3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-
methoxypyrimidin-4-yl]phenoxy]acetonitrile 885066-93-3P,
[3-[6-[[2-(2-Chloro-6-fluorophenyl)ethyl]amino]-2-methoxypyrimidin-4-
yl]phenoxy]acetonitrile 885066-94-4P, 3-[6-[[2-(2-Chloro-6-
fluorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]phenol
885066-99-9P, 2-[3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-
methoxypyrimidin-4-yl]phenoxy]-2-methylpropionic acid ethyl ester
885067-01-6P, 2-Chloro-5-[2-methoxy-6-[[2-(4-
methoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzoic acid ethyl ester
885067-02-7P, [2-(4-Methoxyphenyl)ethyl][2-methoxy-6-[3-(1H-
tetrazol-5-yl)phenyl]pyrimidin-4-yl]amine 885067-03-8P,
3-[2-Methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyrimidin-4-
yl]benzonitrile 885067-05-0P, [3-[2-Methoxy-6-[[2-(4-
methoxyphenyl)ethyl]amino]pyrimidin-4-yl]phenyl]acetonitrile
885067-07-2P, 2-Methoxy-5-[2-methoxy-6-[[2-(4-
methoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzonitrile 885067-09-4P
, 3-[2-Methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzoic
acid 885067-11-8P, 3-[6-[[2-(3,4-Dimethoxyphenyl)ethyl]amino]-2-
methoxypyrimidin-4-yl]benzoic acid 885067-12-9P,
2-Fluoro-5-[2-methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyrimidin-4-
yl]benzaldehyde oxime 885067-14-1P, 2-Methoxy-5-[2-methoxy-6-[[2-
(4-methoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzaldehyde oxime
885067-21-0P, [6-(3-Aminomethyl-4-fluorophenyl)-2-methoxypyrimidin-
4-y1][2-(4-methoxyphenyl)ethyl]amine 885067-42-5P,
3-[2-Methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzamide
885067-43-6P, 1-[3-[2-Methoxy-6-[[2-(4-
methoxyphenyl)ethyl]amino]pyrimidin-4-yl]phenyl]ethanone
885068-16-6P, [3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-
methoxypyrimidin-4-yl]benzoylamino]acetic acid ethyl ester
885068-69-9P, 4-[3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-
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methoxypyrimidin-4-yl]phenyl]tetrahydropyran-4-carboxylic acid 885068-74-6P 885068-81-5P, [3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]phenyl]acetonitrile 885068-82-6P, [3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]phenyl]difluoroacetonitrile 885069-33-0P, 2-[3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]-4-fluorophenyl]-2-methylpropionic acid

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; preparation of aminopyrimidines as prostaglandin D2 receptor antagonists)

RN 885066-02-4 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} & \text{F} \\ \text{NC} & \text{NH-} \text{CH}_2\text{--}\text{CH}_2 \end{array}$$

RN 885066-03-5 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \mathsf{OMe} \\ \mathsf{N} \\ \mathsf{N} \\ \mathsf{NH-CH}_2-\mathsf{CH}_2 \\ \end{array}$$

RN 885066-05-7 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \hline \\ \text{N} \\ \text{N} \\ \text{NH-CH}_2\text{-CH}_2 \\ \hline \\ \text{OMe} \\ \end{array}$$

RN 885066-10-4 CAPLUS

$$\begin{array}{c|c} \text{OMe} \\ \\ \text{N} \\ \text{NH-CH}_2\text{-CH}_2 \end{array}$$

RN 885066-29-5 CAPLUS

CN Benzaldehyde, 3-[2-methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 885066-30-8 CAPLUS

CN Benzenemethanol, 3-[6-[[2-(2-chloro-6-fluorophenyl)ethyl]amino]-2-methoxy-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{OMe} \\ \text{C1} \\ \text{N} \\ \text{N} \\ \text{NH- CH}_2 - \text{CH}_2 \\ \end{array}$$

RN 885066-31-9 CAPLUS

CN Benzaldehyde, 3-[6-[[2-(2-chloro-6-fluorophenyl)ethyl]amino]-2-methoxy-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 885066-50-2 CAPLUS

RN 885066-61-5 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \\ \text{N} \\ \\ \text{NH-} \\ \text{CH}_2 - \text{CH}_2 \end{array} \\ \begin{array}{c|c} \text{OMe} \\ \\ \end{array}$$

RN 885066-63-7 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 885066-65-9 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 885066-67-1 CAPLUS

$$\begin{array}{c|c} & \text{OMe} \\ & \text{Me} \\ & \text{HO}_2\text{C} - \text{C} \\ & \text{Me} \end{array} \qquad \begin{array}{c} \text{N} \\ & \text{N} \\ & \text{NH} - \text{CH}_2 - \text{CH}_2 \\ & \text{C1} \end{array}$$

RN 885066-68-2 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885066-71-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

MeO NH-CH₂-CH₂OMe

RN 885066-81-9 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885066-86-4 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885066-87-5 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \text{O} \\ \text{MeO-C-CH}_2\text{-O} \end{array} \\ \begin{array}{c|c} \text{OMe} \\ \text{NH-CH}_2\text{-CH}_2 \end{array}$$

RN 885066-89-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885066-92-2 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \text{NC-CH}_2\text{-O} \\ \end{array} \begin{array}{c|c} \text{NN} \\ \text{NH-CH}_2\text{-CH}_2 \\ \end{array} \begin{array}{c|c} \text{C1} \\ \text{C1} \\ \end{array}$$

RN 885066-93-3 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} & \text{C1} \\ \hline N & N \\ NC-CH_2-O & NH-CH_2-CH_2 \\ \hline \end{array}$$

RN 885066-94-4 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885066-99-9 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} & \text{OMe} \\ \hline \text{O Me} & \text{N} \\ \hline \text{EtO-C-C-O} & \text{NH-CH}_2\text{-CH}_2 \\ \hline \text{Me} & \text{Cl} \\ \end{array}$$

RN 885067-01-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885067-02-7 CAPLUS

$$\begin{array}{c|c} \text{OMe} \\ \\ N \\ N \\ \end{array} \begin{array}{c} \text{N} \\ N \\ \text{N} \end{array} \begin{array}{c} \text{OMe} \\ \\ N \\ \text{N} \end{array} \begin{array}{c} \text{OMe} \\ \\ N \\ \text{N} \end{array}$$

RN 885067-03-8 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

 $\begin{array}{c|c} \text{OMe} \\ \text{NC} & \text{NH-} \text{CH}_2\text{-}\text{CH}_2 \\ \end{array}$

RN 885067-05-0 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \\ \text{NC-} \text{CH}_2 \\ \end{array} \\ \text{NH-} \text{CH}_2 \\ \text{-} \text{CH}_2 \\ \end{array}$$

RN 885067-07-2 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 885067-09-4 CAPLUS

CN Benzoic acid, 3-[2-methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OMe} \\ \text{NO}_2\text{C} \\ \hline \\ \text{NH-CH}_2\text{-CH}_2 \\ \hline \end{array}$$

RN 885067-11-8 CAPLUS

CN Benzoic acid, 3-[6-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-2-methoxy-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \mathsf{CO_2H} & \mathsf{OMe} & \mathsf{OMe} \\ \hline \\ \mathsf{N} & \mathsf{N} \\ \hline \\ \mathsf{NH-CH_2-CH_2} \end{array}$$

RN 885067-12-9 CAPLUS

CN Benzaldehyde, 2-fluoro-5-[2-methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]-, oxime (9CI) (CA INDEX NAME)

MeO
$$CH_2-CH_2-NH$$
 $HO-N=CH$

RN 885067-14-1 CAPLUS

CN Benzaldehyde, 2-methoxy-5-[2-methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]-, oxime (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OMe} \\ \\ \text{N} \\ \\ \text{N} \\ \\ \text{N} \\ \\ \text{N} \\ \\ \text{OMe} \\ \\ \text{HO-N-CH} \end{array}$$

RN 885067-21-0 CAPLUS

CN 4-Pyrimidinamine, 6-[3-(aminomethyl)-4-fluorophenyl]-2-methoxy-N-[2-(4-methoxyphenyl)ethyl]- (9CI) (CA INDEX NAME)

RN 885067-42-5 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ & \text{N} \\ \text{NH-CH}_2\text{-CH}_2 \\ & \text{OMe} \\ \\ & \text{OMe} \\ \end{array}$$

RN 885067-43-6 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 885068-16-6 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & \text{OMe} \\ & \text{N} & \text{N} \\ & \text{Eto-C-CH}_2-\text{NH-C} \\ & \text{O} & \text{O} \end{array}$$

RN 885068-69-9 CAPLUS

$$\begin{array}{c|c} \text{C1} & \text{OMe} \\ \hline \\ \text{C1} & \text{CH}_2\text{-}\text{CH}_2\text{-}\text{NH} \\ \hline \end{array}$$

RN 885068-74-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \\ \text{N} \\ \text{N} \\ \text{NH-CH}_2\text{-CH}_2 \\ \\ \text{Cl} \end{array}$$

RN 885068-81-5 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \text{NC-CH}_2 \\ \end{array} \begin{array}{c} \text{NH-CH}_2\text{-CH}_2 \\ \text{Cl} \\ \end{array}$$

RN 885068-82-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885069-33-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & \text{Me} \\ & \text{MeO} & \text{Me-C-CO}_2\text{H} \\ \hline & \text{CH}_2\text{-CH}_2\text{-NH} \\ & \text{Cl} & \text{F} \\ \end{array}$$

885066-07-9P, 3-[2-Methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyri IT midin-4-yl]-N-methylbenzenesulfonamide 885066-08-0P, N-Ethyl-3-[2-methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyrimidin-4yl]benzenesulfonamide 885066-09-1P, N-(Methoxycarbonyl)-3-[2methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyrimidin-4yl]benzenesulfonamide 885066-12-6P, N-[3-[2-Methoxy-6-[[2-(4trifluoromethoxyphenyl)ethyl]amino]pyrimidin-4-yl]phenyl]acetamide **885066-13-7P**, N-[3-[2-Methoxy-6-[[2-(4methoxyphenyl)ethyl]amino]pyrimidin-4-yl]phenyl]acetamide **885066-14-8P**, [3-[2-Methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyr imidin-4-yl]phenyl]carbamic acid ethyl ester 885066-17-1P, 3-[6-[[2-(2,4-Difluorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]benzoic acid 885066-28-4P, [3-[2-Methoxy-6-[[2-(4methoxyphenyl)ethyl]amino]pyrimidin-4-yl]phenyl]methanol 885066-35-3P, N-[2-[2-Methoxy-6-[[2-(4methoxyphenyl)ethyl]amino]pyrimidin-4-yl]phenyl]methanesulfonamide **885066-36-4P**, 4-[2-Methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyri methoxyphenyl)ethyl]amino]pyrimidin-4-yl]phenyl]ethanone 885066-40-0P, [6-(3-Methylsulfonylphenyl)-2-methoxypyrimidin-4yl][2-(4-methoxyphenyl)ethyl]amine 885066-42-2P, [2-Methoxy-6-[4-(morpholin-4-yl)phenyl]pyrimidin-4-yl][2-(4-yl)phenyl]methoxyphenyl)ethyl]amine 885066-43-3P, [6-(4-Dimethylaminophenyl)-2-methoxypyrimidin-4-yl][2-(4methoxyphenyl)ethyl]amine 885066-46-6P, [2-Methoxy-6-[3-(oxazol-5-yl)phenyl]pyrimidin-4-yl][2-(4-methoxyphenyl)ethyl]amine 885066-49-9P, [6-[4-Fluoro-3-[(2-methoxyethylamino)methyl]phenyl]-2-methoxypyrimidin-4-yl][2-(4-methoxyphenyl)ethyl]amine monohydrochloride 885066-51-3P, 4-[2-[[3-[2-Methoxy-6-[[2-(4methoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzyl]amino]ethyl]phenol monohydrochloride 885066-52-4P, N-[2-Fluoro-5-[2-methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzyl]-N',N'-dimethylethane-1,2-diamine monohydrochloride 885066-60-4P, 3-[2-Methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyrimidin-4-yl]phenol hydrochloride 885066-62-6P, 3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2methoxypyrimidin-4-yl]benzoic acid monohydrochloride 885066-64-8P , 3-[6-[[2-(2-Chloro-6-fluorophenyl)ethyl]amino]-2-methoxypyrimidin-4yl]benzoic acid monohydrochloride 885066-66-0P, 2-[3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4yl]phenyl]-2-methylpropionic acid monohydrochloride 885066-70-6P , 3-[6-[[2-(3,4-Dimethoxyphenyl)ethyl]amino]-2-methylsulfanylpyrimidin-4yl]benzoic acid 885066-73-9p, [2-(3,4-Dimethoxyphenyl)ethyl][6-(3,4-dimethoxyphenyl)-2-isopropoxypyrimidin-4-yl]amine 885066-75-1P, [6-(3,4-Dimethoxyphenyl)-2-ethoxypyrimidin-4-yl][2-(3,4-dimethoxyphenyl)ethyl]amine 885066-76-2P,

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[2-Ethyl-6-(3-methoxyphenyl)pyrimidin-4-yl][2-(4-methoxyphenyl)ethyl]amine
885066-78-4P, 6-(3-Methoxyphenyl)-N'-[2-(4-methoxyphenyl)ethyl]-
N, N-dimethylpyrimidine-2, 4-diamine monohydrochloride 885066-79-5P
, 2-Fluoro-5-[2-methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyrimidin-4-
yl]benzoic acid 885066-80-8P, 2-Methoxy-5-[2-methoxy-6-[[2-(4-
methoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzoic acid 885066-88-6P
, [3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-
yl]phenoxy]acetic acid methyl ester 885066-95-5P,
2-[3-[2-Methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyrimidin-4-yl]phenoxy]-
2-methylpropionic acid 885066-96-6P, [3-[2-Methoxy-6-[[2-(4-
methoxyphenyl)ethyl]amino]pyrimidin-4-yl]phenoxy]acetic acid
885066-98-8P, 2-[3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-
methoxypyrimidin-4-yl]phenoxy]-2-methylpropionic acid 885067-00-5P
, 2-Chloro-5-[2-methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyrimidin-4-
yl]benzoic acid monohydrochloride 885067-04-9P,
[2-(4-Methoxyphenyl)ethyl][2-methoxy-6-[3-[(1H-tetrazol-5-
yl)methyl]phenyl]pyrimidin-4-yl]amine monohydrochloride
885067-06-1P, [2-Methoxy-6-[4-methoxy-3-(1H-tetrazol-5-
yl)phenyl]pyrimidin-4-yl][2-(4-methoxyphenyl)ethyl]amine
885067-08-3P, N-[3-[2-Methoxy-6-[[2-(4-
methoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzoyl]methanesulfonamide
885067-10-7P, 3-[6-[[2-(3,4-Dimethoxyphenyl)ethyl]amino]-2-
methoxypyrimidin-4-yl]-N-[2-(pyrrolidin-1-yl)ethyl]benzamide
885067-13-0P, 3-[2-Methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyri
midin-4-yl]benzaldehyde oxime 885067-19-6P, [6-(3-Aminomethyl-4-
fluorophenyl)-2-methoxypyrimidin-4-yl][2-(4-methoxyphenyl)ethyl]amine
monohydrochloride 885067-20-9P, N-[2-Fluoro-5-[2-methoxy-6-[[2-
(4-methoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzyl]-2-methoxyacetamide
monohydrochloride 885067-29-8P, 3-[[3-[6-[[2-(2,4-
Dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]phenoxy]methyl]-4H-
[1,2,4]oxadiazol-5-one monohydrochloride 885067-31-2P,
3-[3-[6-[[2-(2-Chloro-6-fluorophenyl)ethyl]amino]-2-methoxypyrimidin-4-
yl]benzyl]-4H-[1,2,4]oxadiazol-5-one monohydrochloride
885067-34-5P, 3-[[3-[6-[[2-(2-Chloro-6-fluorophenyl)ethyl]amino]-2-
methoxypyrimidin-4-yl]phenoxy]methyl]-4H-[1,2,4]oxadiazol-5-one
monohydrochloride 885067-36-7P, 3-[2-Methoxy-6-[[2-(4-
trifluoromethoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzoic acid
885067-39-0P, [6-(Biphenyl-4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-methoxypyrimidin-4-yl][2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(3,4-yl)-2-(
dimethoxyphenyl)ethyl]amine 885067-40-3P, 3-[6-[[2-(4-
Fluorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]benzoic acid
hydrochloride 885067-44-7P, 3-[6-[[2-(4-
Chlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]benzoic acid
monohydrochloride 885067-48-1P, 2-[2-Methoxy-6-[[2-(4-
methoxyphenyl)ethyl]amino]pyrimidin-4-yl]phenol 885067-52-7P,
[2-Methoxy-6-[3-(3-methyl-[1,2,4]oxadiazol-5-yl)phenyl]pyrimidin-4-yl][2-methoxy-6-[3-(3-methyl-[1,2,4]oxadiazol-5-yl)phenyl]pyrimidin-4-yl][2-methoxy-6-[3-(3-methyl-[1,2,4]oxadiazol-5-yl)phenyl]pyrimidin-4-yl][2-methoxy-6-[3-(3-methyl-[1,2,4]oxadiazol-5-yl)phenyl]pyrimidin-4-yl][2-methoxy-6-[3-(3-methyl-[1,2,4]oxadiazol-5-yl)phenyl]pyrimidin-4-yl][2-methoxy-6-[3-(3-methyl-[1,2,4]oxadiazol-5-yl)phenyl]pyrimidin-4-yl][2-methoxy-6-[3-(3-methyl-[1,2,4]oxadiazol-5-yl)phenyl]pyrimidin-4-yl][2-methoxy-6-[3-(3-methyl-[1,2,4]oxadiazol-5-yl)phenyl]pyrimidin-4-yl][2-methyl-[1,2,4]oxadiazol-5-yl)phenyl]pyrimidin-4-yl][2-methyl-[1,2,4]oxadiazol-5-yl)phenyl]pyrimidin-4-yl][2-methyl-[1,2,4]oxadiazol-5-yl]phenyl]pyrimidin-4-yl][2-methyl-[1,2,4]oxadiazol-5-yl]phenyl]pyrimidin-4-yl][2-methyl-[1,2,4]oxadiazol-5-yl]phenyl]pyrimidin-4-yl][2-methyl-[1,2,4]oxadiazol-5-yl]phenyl]pyrimidin-4-yl][2-methyl-[1,2,4]oxadiazol-5-yl]phenyl]pyrimidin-4-yl][2-methyl-[1,2,4]oxadiazol-5-yl]phenyl]pyrimidin-4-yl][2-methyl-[1,2,4]oxadiazol-5-yl]phenyl]pyrimidin-4-yl][2-methyl-[1,2,4]oxadiazol-5-yl]phenyl]pyrimidin-4-yl][2-methyl-[1,2,4]oxadiazol-5-yl]phenyl]pyrimidin-4-yl][2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4]oxadiazol-5-yl]phenyl[2-methyl-[1,2,4
(4-methoxyphenyl)ethyl]amine 885067-54-9P, [2-Methoxy-6-[3-(5-
methyl-4H-[1,2,4]triazol-3-yl) phenyl] pyrimidin-4-yl] [2-(4-
methoxyphenyl)ethyl]amine 885067-55-0P, [2-Methoxy-6-[3-(3-
methylisoxazol-5-yl)phenyl]pyrimidin-4-yl][2-(4-methoxyphenyl)ethyl]amine
885067-56-1P 885067-57-2P, [2-(3-Fluoro-4-
methoxyphenyl)ethyl][2-methoxy-6-[3-(2H-tetrazol-5-yl)phenyl]pyrimidin-4-
yl]amine 885067-58-3P, 1-Ethyl-3-[3-[2-methoxy-6-[[2-(4-
methoxyphenyl)ethyl]amino]pyrimidin-4-yl]phenyl]urea 885067-63-0P
, [2-Methoxy-6-(3-methoxyphenyl)pyrimidin-4-yl][2-(4-
nitrophenyl)ethyl]amine 885067-65-2P, [2-Methoxy-6-(3-
methoxyphenyl)pyrimidin-4-yl][2-(4-trifluoromethoxyphenyl)ethyl]amine
885067-66-3P, [2-(2-Chloro-6-fluorophenyl)ethyl][2-methoxy-6-(3-
methoxyphenyl)pyrimidin-4-yl]amine hydrochloride 885067-72-1P,
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[2-(4-Aminophenyl)ethyl][2-methoxy-6-(3-methoxyphenyl)pyrimidin-4-yl]amine
monohydrochloride 885067-73-2P, (4-Methoxybenzyl)[2-methoxy-6-(3-
methoxyphenyl)pyrimidin-4-yl]amine monohydrochloride 885067-74-3P
  [2-Methoxy-6-(3-methoxyphenyl)pyrimidin-4-yl](3-phenylpropyl)amine
monohydrochloride 885067-77-6P, [2-Methoxy-6-(3-
methoxyphenyl)pyrimidin-4-yl][2-(4-methoxyphenyl)ethyl]amine
885067-86-7P, 3-[6-[[2-(2,2-Difluorobenzodioxol-5-yl)ethyl]amino]-
2-methoxypyrimidin-4-yl]benzoic acid 885067-91-4P,
yl]phenyl]acetamide monohydrochloride 885067-92-5P,
[2-[4-(Difluoromethoxy)phenyl]ethyl][6-(3-methylsulfonylphenyl)-2-
methoxypyrimidin-4-yl]amine monohydrochloride 885067-93-6P,
[2-(2,4-Dichlorophenyl)] [2-methyl-6-[3-[1-methyl-1-(1H-tetrazol-5-1]]
yl)ethyl]phenyl]pyrimidin-4-yl]amine monohydrochloride
885067-99-2P, 2-[3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-
methoxypyrimidin-4-yl]phenyl]propionic acid monohydrochloride
885068-01-9P, 2-[3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-
methoxypyrimidin-4-yl]phenyl]-2-methylpropionic acid 1-
(ethoxycarbonyloxy)ethyl ester monohydrochloride 885068-02-0P,
2-[3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-
yl]phenyl]-2-methylpropionic acid 2-dimethylaminoethyl ester
dihydrochloride 885068-11-1P, 3-[6-[[2-(2,6-
Dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]benzoic acid
885068-12-2P 885068-13-3P, [[3-[6-[[2-(2-Chloro-6-
fluorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]benzyl]oxy]acetic acid
885068-14-4P 885068-17-7P, [3-[6-[[2-(2,4-
Dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]benzoylamino]acetic
acid 885068-18-8P, Ethylcarbamic acid 3-[6-[[2-(2,4-
dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]phenyl ester
885068-27-9P 885068-28-0P, N-[2-[3-[6-[[2-(2-Fluoro-4-
trifluoromethylphenyl)ethyl]amino]-2-methoxypyrimidin-4-
yl]phenyl]ethyl]acetamide monohydrochloride 885068-29-1P,
[2-(2-Fluoro-4-trifluoromethylphenyl)ethyl][2-methoxy-6-[3-
[(oxiranyl)methoxy]phenyl]pyrimidin-4-yl]amine 885068-33-7P,
2-[3-[2-Methoxy-6-[[2-[4-(5-methyl-[1,3,4]oxadiazol-2-
yl)phenyl]ethyl]amino]pyrimidin-4-yl]phenyl]-2-methylpropionic acid
885068-37-1P 885068-45-1P, 2-[2-Fluoro-5-[2-methoxy-6-
[[2-(4-trifluoromethoxyphenyl)ethyl]amino]pyrimidin-4-yl]phenyl]-2-
methylpropionic acid 885068-61-1P, 1-[3-[6-[[2-(2,4-
Dichlorophenyl) ethyl] amino] -2-methoxypyrimidin-4-
yl]phenyl]cyclopentanecarboxylic acid monohydrochloride
885068-63-3P, 3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-
methoxypyrimidin-4-yl]benzoic acid 2-(morpholin-4-yl)ethyl ester
885068-64-4P, 3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-
methoxypyrimidin-4-yl]benzoic acid 2-(4-methylpiperazin-1-yl)ethyl ester
885068-65-5P, 3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-
methoxypyrimidin-4-yl]benzoic acid ethyl ester 885068-66-6P,
[3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-
yl]phenyl]methanol 885068-67-7P, 1-[3'-Chloro-4'-[2-[[6-(3-
hydroxymethylphenyl)-2-methoxypyrimidin-4-yl]amino]ethyl]biphenyl-3-
yl]methanol 885068-68-8P, 2-[3-[6-[[2-(2,4-
Dichlorophenyl) ethyl] amino] -2-methoxypyrimidin-4-yl] phenyl] -2-
methylpropionic acid methyl ester 885068-72-4P,
N-[4-3-6-[2-4] height of N-[4-6] methoxypyrimidin-4-
yl]phenyl]tetrahydropyran-4-yl]carbonyl]methanesulfonamide
885068-73-5P, 4-[3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-
methoxypyrimidin-4-yl]phenyl]tetrahydropyran-4-carboxylic acid ethyl ester
885068-78-0P 885068-79-1P 885068-83-7P,
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[2-(2,4-Dichlorophenyl)ethyl][6-[3-[difluoro(1H-tetrazol-5-
yl)methyl]phenyl]-2-methoxypyrimidin-4-yl]amine 885068-88-2P,
N-[[4-[3-[2-Methoxy-6-[[2-(4-trifluoromethoxyphenyl)ethyl]amino]pyrimidin-
4-y1]phenyl]tetrahydropyran-4-y1]carbonyl]methanesulfonamide
885068-90-6P, 4-[3-[2-Methoxy-6-[[2-(4-
trifluoromethoxyphenyl)ethyl]amino]pyrimidin-4-yl]phenyl]tetrahydropyran-4-
carboxylic acid methyl ester 885068-91-7p, 2-[3-[6-[2-(2,4-
Dichlorophenyl)ethyl]amino]-2-(methoxymethyl)pyrimidin-4-yl]phenyl]-2-
methylpropionic acid 885068-93-9P, 2-[3-[6-[[2-(2,4-
Dichlorophenyl)ethyl]amino]-2-hydroxymethylpyrimidin-4-yl]phenyl]-2-
methylpropionic acid 885069-05-6P, 2-[3-[6-[[2-(2,4-
Dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]phenyl]-2-
methylpropionic acid 2,3-dihydroxypropyl ester 885069-12-5P,
2-[3-[6-[(Benzofuran-5-ylmethyl)amino]-2-methoxypyrimidin-4-yl]phenyl]-2-
methylpropionic acid 885069-16-9P, Ethanesulfonic acid
N-[2-[3-[6-[2-(2,4-dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-
yl]phenyl]-2-methylpropionyl]amide 885069-17-0P,
N-[2-[3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-
yl]phenyl]-2-methylpropionyl]-1-phenylmethanesulfonamide
885069-18-1P, 2-[3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-
methoxypyrimidin-4-yl]phenyl]-2-methyl-1-(morpholin-4-yl)propan-1-one
885069-19-2P, 2-[3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-
methoxypyrimidin-4-yl]phenyl]-N-(tetrahydropyran-4-yl)isobutyramide
885069-20-5P, 2-[3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-
methoxypyrimidin-4-yl]phenyl]-N-(1H-tetrazol-5-yl)isobutyramide
885069-28-3P, 2-[2-Chloro-5-[6-[[2-(2,4-
dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]phenyl]propan-2-ol
885069-31-8P, 2-[3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-
methoxypyrimidin-4-yl]-4-fluorophenyl]-2-methylpropionic acid
monohydrochloride 885069-35-2P, [6-[4-Fluoro-3-[(2-
methoxyethylamino)methyl]phenyl]-2-methoxypyrimidin-4-yl][2-(4-
methoxyphenyl)ethyl]amine 885069-36-3p, 4-[2-[[3-[2-Methoxy-6-
[[2-(4-methoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzyl]amino]ethyl]phenol
885069-37-4P, N-[2-Fluoro-5-[2-methoxy-6-[[2-(4-
methoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzyl]-N',N'-dimethylethane-1,2-
diamine 885069-38-5P, 6-(3-Methoxyphenyl)-N'-[2-(4-
methoxyphenyl)ethyl]-N,N-dimethylpyrimidine-2,4-diamine
885069-39-6P, 2-Chloro-5-[2-methoxy-6-[[2-(4-
methoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzoic acid 885069-40-9P
, [2-(4-Methoxyphenyl)ethyl][2-methoxy-6-[3-[(1H-tetrazol-5-
yl)methyl]phenyl]pyrimidin-4-yl]amine 885069-41-0P,
N-[2-Fluoro-5-[2-methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyrimidin-4-
yl]benzyl]-2-methoxyacetamide 885069-42-1p, 3-[[3-[6-[[2-(2,4-
Dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]phenoxy]methyl]-4H-
[1,2,4]oxadiazol-5-one 885069-43-2P, 3-[3-[6-[[2-(2-Chloro-6-
fluorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]benzyl]-4H-
[1,2,4]oxadiazol-5-one 885069-44-3P, 3-[[3-[6-[[2-(2-Chloro-6-
fluorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]phenoxy]methyl]-4H-
[1,2,4]oxadiazol-5-one 885069-45-4P, 3-[6-[[2-(4-
Fluorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]benzoic acid
885069-46-5P, 3-[6-[[2-(4-Chlorophenyl)ethyl]amino]-2-
methoxypyrimidin-4-yl]benzoic acid 885069-47-6P,
[2-(2-Chloro-6-fluorophenyl)ethyl][2-methoxy-6-(3-methoxyphenyl)pyrimidin-
4-y1] amine 885069-52-3P, [2-(4-Aminophenyl)ethyl] [2-methoxy-6-(3-
methoxyphenyl)pyrimidin-4-yl]amine 885069-53-4P,
(4-Methoxybenzyl) [2-methoxy-6-(3-methoxyphenyl)pyrimidin-4-yl]amine
885069-54-5P, [2-Methoxy-6-(3-methoxyphenyl)pyrimidin-4-yl](3-
phenylpropyl)amine 885069-55-6P, N-[3-[6-[[2-[4-
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(Difluoromethoxy)phenyl]ethyl]amino]-2-methoxypyrimidin-4-
yl]phenyl]acetamide 885069-56-7P, [2-[4-
(Difluoromethoxy)phenyl]ethyl][6-(3-methylsulfonylphenyl)-2-
methoxypyrimidin-4-yl]amine 885069-57-8P,
[2-(2,4-Dichlorophenyl)] [2-methyl-6-[3-[1-methyl-1-(1H-tetrazol-5-1]]
yl)ethyl]phenyl]pyrimidin-4-yl]amine 885069-60-3P,
2-[3-[6-[2-(2,4-Dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-
yl]phenyl]propionic acid 885069-61-4P, 2-[3-[6-[[2-(2,4-
Dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]phenyl]-2-
methylpropionic acid 1-(ethoxycarbonyloxy)ethyl ester 885069-62-5P
, 2-[3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-
yl]phenyl]-2-methylpropionic acid 2-dimethylaminoethyl ester
885069-64-7P, N-[2-[3-[6-[[2-(2-Fluoro-4-
trifluoromethylphenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]phenyl]ethyl]-2-
methoxyacetamide 885069-65-8P, N-[2-[3-[6-[[2-(2-Fluoro-4-
trifluoromethylphenyl)ethyl]amino]-2-methoxypyrimidin-4-
yl]phenyl]ethyl]acetamide 885069-67-0P, 1-[3-[6-[[2-(2,4-
Dichlorophenyl) ethyl] amino] -2-methoxypyrimidin-4-
yl]phenyl]cyclopentanecarboxylic acid 885069-72-7P,
3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]phenol
hydrochloride
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (drug candidate; preparation of aminopyrimidines as prostaglandin D2
   receptor antagonists)
885066-07-9 CAPLUS
INDEX NAME NOT YET ASSIGNED
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RN 885066-08-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN

CN

RN 885066-09-1 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & \text{OMe} \\ \hline \\ \text{MeO-C-NH-S} \\ \hline \\ \text{O} & \text{O} \end{array}$$

RN 885066-12-6 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 885066-13-7 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 885066-14-8 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \hline \\ \text{O} \\ \hline \\ \text{EtO-C-NH} \end{array} \\ \text{NH-CH}_2\text{-CH}_2 \\ \hline \end{array}$$

RN 885066-17-1 CAPLUS

OMe
$$NH-CH_2-CH_2$$

$$F$$

$$CO_2H$$

RN 885066-28-4 CAPLUS

CN Benzenemethanol, 3-[2-methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OMe} \\ \hline \\ \text{N} \\ \text{NH-CH}_2\text{-CH}_2 \end{array} \\ \begin{array}{c|c} \text{OMe} \\ \\ \text{OMe} \\ \end{array}$$

RN 885066-35-3 CAPLUS

CN Methanesulfonamide, N-[2-[2-methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]- (9CI) (CA INDEX NAME)

RN 885066-36-4 CAPLUS

CN Benzamide, 4-[2-methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]-4-pyrimidinyl](9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{O} & \text{OMe} \\ \text{H}_2\text{N}-\text{C} & \text{N} & \text{N} \\ & \text{N} & \text{N} + \text{CH}_2-\text{CH}_2 \end{array}$$

RN 885066-39-7 CAPLUS

CN Ethanone, 1-[4-[2-methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OMe} \\ \text{N} \\ \text{N} \\ \text{NH-CH}_2\text{-CH}_2 \\ \end{array}$$

RN 885066-40-0 CAPLUS

CN 4-Pyrimidinamine, 2-methoxy-N-[2-(4-methoxyphenyl)ethyl]-6-[3-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

RN 885066-42-2 CAPLUS

CN 4-Pyrimidinamine, 2-methoxy-N-[2-(4-methoxyphenyl)ethyl]-6-[4-(4-morpholinyl)phenyl]- (9CI) (CA INDEX NAME)

RN 885066-43-3 CAPLUS

CN 4-Pyrimidinamine, 6-[4-(dimethylamino)phenyl]-2-methoxy-N-[2-(4-methoxyphenyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OMe} \\ \text{Me}_2\text{N} \\ \text{N} \\ \text{NH-CH}_2\text{-CH}_2 \\ \end{array}$$

RN 885066-46-6 CAPLUS

CN 4-Pyrimidinamine, 2-methoxy-N-[2-(4-methoxyphenyl)ethyl]-6-[3-(5-oxazolyl)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

RN 885066-49-9 CAPLUS CN INDEX NAME NOT YET ASSIGNED

● HCl

RN 885066-51-3 CAPLUS CN INDEX NAME NOT YET ASSIGNED

PAGE 1-A

● HCl

PAGE 1-B

RN 885066-52-4 CAPLUS

HCl

RN 885066-60-4 CAPLUS CN INDEX NAME NOT YET ASSIGNED

● HCl

RN 885066-62-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

● HCl

RN 885066-64-8 CAPLUS CN INDEX NAME NOT YET ASSIGNED

HCl

RN 885066-66-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & \text{OMe} \\ & \text{N} \\ \text{HO}_2\text{C} - \text{C} \\ & \text{Me} \end{array} \qquad \begin{array}{c} \text{OMe} \\ & \text{N} \\ & \text{NH} - \text{CH}_2 - \text{CH}_2 \\ & \text{C1} \end{array}$$

HCl

RN 885066-70-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885066-73-9 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885066-75-1 CAPLUS

RN 885066-76-2 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 885066-78-4 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

● HCl

RN 885066-79-5 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 885066-80-8 CAPLUS

RN 885066-88-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \text{O} \\ \text{MeO-C-CH}_2\text{-O} \\ \end{array}$$

RN 885066-95-5 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \text{Me} \\ \text{HO}_2\text{C}-\text{C}-\text{O} \\ \text{Me} \end{array}$$

RN 885066-96-6 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \hline \\ \text{N} \\ \text{NH-CH}_2\text{-CH}_2 \\ \end{array}$$

RN 885066-98-8 CAPLUS

$$\begin{array}{c|c} \text{Me} & \text{OMe} \\ \text{Me} & \text{N} & \text{N} \\ \text{HO}_2\text{C}-\text{C}-\text{O} & \text{NH}-\text{CH}_2-\text{CH}_2 \\ \text{Me} & \text{C1} \end{array}$$

RN 885067-00-5 CAPLUS CN INDEX NAME NOT YET ASSIGNED

HCl

RN 885067-04-9 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c} \text{OMe} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{H} \end{array} \\ \begin{array}{c} \text{OMe} \\ \text{N} \\ \text{N} \\ \text{H} \end{array} \\ \begin{array}{c} \text{OMe} \\ \text{N} \\ \text{OMe} \\ \text{N} \\ \text$$

HCl

RN 885067-06-1 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c} \text{MeO} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{H} \end{array} \qquad \begin{array}{c} \text{OMe} \\ \text{N} \\ \text{N} \\ \text{H} \end{array}$$

RN 885067-08-3 CAPLUS

CN Benzamide, 3-[2-methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]-N-(methylsulfonyl)- (9CI) (CA INDEX NAME)

RN 885067-10-7 CAPLUS

CN Benzamide, 3-[6-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-2-methoxy-4-pyrimidinyl]-N-[2-(1-pyrrolidinyl)ethyl]- (9CI) (CA INDEX NAME)

RN 885067-13-0 CAPLUS

CN Benzaldehyde, 3-[2-methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]-, oxime (9CI) (CA INDEX NAME)

OMe NH-CH₂-CH₂

$$NH-CH2-CH2$$

RN 885067-19-6 CAPLUS

CN 4-Pyrimidinamine, 6-[3-(aminomethyl)-4-fluorophenyl]-2-methoxy-N-[2-(4-methoxyphenyl)ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 885067-20-9 CAPLUS

CN Acetamide, N-[[2-fluoro-5-[2-methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-2-methoxy-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 885067-29-8 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c}
\text{OMe} \\
\text{N} \\
\text{N} \\
\text{NH- CH}_2 - \text{CH}_2
\end{array}$$

HCl

RN 885067-31-2 CAPLUS CN INDEX NAME NOT YET ASSIGNED

OMe
$$CH_2$$

$$NH-CH_2-CH_2$$

$$C1$$

● HCl

RN 885067-34-5 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c}
OMe \\
N \\
N \\
NH-CH_2-CH_2
\end{array}$$

HCl

RN 885067-36-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \\ \text{N} \\ \text{NH-} \\ \text{CH}_2 - \text{CH}_2 \end{array}$$

RN 885067-39-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} & \text{OMe} \\ \hline \text{NN} & \text{NN} \\ \hline \text{NH-CH}_2\text{-CH}_2 \\ \hline \end{array}$$

RN 885067-40-3 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \text{N} & \text{N} \\ \text{NH-CH}_2\text{-CH}_2 \\ \end{array}$$

HCl

RN 885067-44-7 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

HCl

RN 885067-48-1 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c} \text{OMe} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{HO} \\ \end{array}$$

RN 885067-52-7 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \\ \text{N} \\ \\ \text{N} \\ \\ \text{O} \end{array}$$

RN 885067-54-9 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 885067-55-0 CAPLUS

$$\begin{array}{c} \text{Me} \\ \text{MeO} \\ \\ \text{N} \\ \text{N} \\ \text{N} \\ \\ \text{MeO} \\ \\ \\ \text{MeO} \\ \\ \text{Me$$

RN 885067-56-1 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{MeO} & \text{OMe} \\ & \text{N} & \text{N} \\ & \text{CH}_2\text{-}\text{CH}_2\text{-}\text{NH} \\ & \text{MeO} \\ & \text{MeO} \\ & \text{N} \\ & \text{N} \\ & \text{N} \\ & \text{MeO} \\ & \text{N} \\ & \text$$

RN 885067-57-2 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} & \text{F} \\ \text{N} & \text{N} \\ \text{N} & \text{N} \\ \text{N} & \text{N} \\ \text{N} & \text{H} \end{array}$$

RN 885067-58-3 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \hline \\ \text{O} \\ \hline \\ \text{EtNH-C-NH} \\ \end{array} \\ \begin{array}{c|c} \text{OMe} \\ \hline \\ \text{NH-CH}_2\text{-CH}_2 \\ \hline \end{array}$$

RN 885067-63-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885067-65-2 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885067-66-3 CAPLUS CN INDEX NAME NOT YET ASSIGNED

● HCl

RN 885067-72-1 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} & & \text{NH}_2 \\ \hline & \text{N} & \text{NH} - \text{CH}_2 - \text{CH}_2 \\ \hline \end{array}$$

HCl

RN 885067-73-2 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

● HCl

RN 885067-74-3 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \\ \text{N} \\ \\ \text{N} \\ \\ \text{N} \\ \\ \text{OMe} \\ \end{array}$$

HCl

RN 885067-77-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \text{N} \\ \text{NH} \\ \text{CH}_2 \\ \text{CH}_2 \end{array} \\ \begin{array}{c|c} \text{OMe} \\ \\ \text{OM$$

RN 885067-86-7 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \text{N} \\ \text{NH-CH}_2\text{-CH}_2 \\ \end{array}$$

RN 885067-91-4 CAPLUS CN INDEX NAME NOT YET ASSIGNED

HCl

RN 885067-92-5 CAPLUS CN INDEX NAME NOT YET ASSIGNED

● HCl

RN 885067-93-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

● HCl

RN 885067-99-2 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \\ \text{N} \\ \text{N} \\ \text{NH-} \\ \text{CH}_2\text{-} \\ \text{CH}_2 \\ \end{array}$$

● HCl

RN 885068-01-9 CAPLUS CN INDEX NAME NOT YET ASSIGNED

● HCl

RN 885068-02-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & \text{OMe} \\ & \text{Me} \\ \text{Me}_2\text{N}-\text{CH}_2-\text{CH}_2-\text{O}-\text{C}-\text{C} \\ & \text{O} \\ \text{O} \\ \text{Me} \end{array}$$

●2 HCl

RN 885068-11-1 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885068-12-2 CAPLUS CN INDEX NAME NOT YET ASSIGNED

OMe
$$N = N + CH_2 - CH_2$$

$$N = N + CH_2 - CH_2$$

Na

RN 885068-13-3 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} & \text{C1} \\ \text{N} & \text{N} \\ \text{HO}_2\text{C}-\text{CH}_2-\text{O}-\text{CH}_2 \end{array}$$

RN 885068-14-4 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} & \text{C1} \\ \text{Me} & \text{N} & \text{N} \\ \text{HO}_2\text{C} - \text{C} & \text{NH} - \text{CH}_2 - \text{CH}_2 \\ & \text{Me} & \text{C1} \\ \end{array}$$

Na

RN 885068-17-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \\ \text{N} \\ \text{N} \\ \text{NH-CH}_2\text{-CH}_2 \\ \\ \text{C1} \\ \end{array}$$

RN 885068-18-8 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885068-27-9 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & \text{OMe} \\ \hline \\ \text{O} \\ \hline \\ \text{MeO-} \text{CH}_2 - \text{C-} \text{NH-} \text{CH}_2 - \text{CH}_2 \\ \hline \end{array}$$

●x HCl

RN 885068-28-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \\ \text{N} \\ \text{NH-CH}_2\text{-CH}_2 \\ \end{array}$$

● HCl

RN 885068-29-1 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$CH_2-O$$
 $NH-CH_2-CH_2$
 CF_3

RN 885068-33-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} & \text{Me} \\ \text{N} & \text{N} & \text{Me} \\ \text{C-CO}_2\text{H} \\ \text{Me} & \text{Me} \end{array}$$

RN 885068-37-1 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c} \text{OMe} \\ \text{N} \\ \text{N} \\ \text{O} \\ \text{Et} \end{array}$$

RN 885068-45-1 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 885068-61-1 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

● HCl

RN 885068-63-3 CAPLUS

RN 885068-64-4 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

PAGE 1-A

PAGE 1-B

__ Me

RN 885068-65-5 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \\ \text{N} \\ \\ \text{N} \\ \\ \text{NH-CH}_2\text{-CH}_2 \\ \\ \\ \text{C1} \\ \end{array}$$

RN 885068-66-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} & \text{C1} \\ \hline \\ \text{HO-CH}_2 & \text{NH-CH}_2\text{-CH}_2 \\ \hline \\ \text{C1} \end{array}$$

RN 885068-67-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} & \text{Cl} \\ \hline & \text{N} \\ \text{HO-CH}_2 \\ \end{array}$$

RN 885068-68-8 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & \text{OMe} \\ & \text{Me} \\ & \text{MeO-C-C} \\ & \text{O Me} \\ \end{array}$$

RN 885068-72-4 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885068-73-5 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885068-78-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & \text{OMe} \\ & \text{O} & \text{O} \\ & \text{Et-S-NH-C-CF}_2 \\ & \text{O} \\ & \text{O} \end{array}$$

RN 885068-79-1 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} & \text{OMe} \\ \hline \\ \text{EtO-C-CF}_2 & \text{NH-CH}_2\text{-CH}_2 \\ \hline \\ \text{C1} \end{array}$$

RN 885068-83-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \\ N \\ N \\ H \end{array} \qquad \begin{array}{c} \text{C1} \\ \\ \text{C1} \end{array}$$

RN 885068-88-2 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885068-90-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885068-91-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & \text{MeO-CH}_2 \\ & \text{Me} \\ & \text{HO}_2\text{C-C} \\ & \text{Me} \end{array} \qquad \begin{array}{c} \text{N} \\ & \text{NH-CH}_2\text{-CH}_2 \\ & \text{C1} \end{array}$$

RN 885068-93-9 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & \text{HO-CH2} \\ & \text{Me} & \text{N} \\ & \text{HO}_2\text{C-C} \\ & \text{Me} \end{array}$$

RN 885069-05-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885069-12-5 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885069-16-9 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} O & Me & N & N \\ \hline \\ Et-S-NH-C-C & NH-CH2-CH2 & C1 \\ \hline \\ O & O & Me & C1 \\ \end{array}.$$

RN 885069-17-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885069-18-1 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885069-19-2 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885069-20-5 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885069-28-3 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885069-31-8 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & \text{Me} \\ & \text{MeO} & \text{Me-C-CO}_2\text{H} \\ \hline \text{Cl} & \text{CH}_2\text{-CH}_2\text{-NH} \\ & \text{F} \end{array}$$

HCl

RN 885069-35-2 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885069-36-3 CAPLUS CN INDEX NAME NOT YET ASSIGNED

PAGE 1-A

PAGE 1-B

RN 885069-37-4 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885069-38-5 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & \text{NMe}_2 \\ & \text{N} \\ & \text{N} \\ & \text{NH-CH}_2\text{-CH}_2 \end{array} \\ \begin{array}{c} \text{OMe} \\ \\ \end{array}$$

RN 885069-39-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885069-40-9 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885069-41-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

Page 73

RN 885069-42-1 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

OMe
$$CH_2-O$$

$$N$$

$$N$$

$$N$$

$$N$$

$$N$$

$$N$$

$$CH_2-CH_2$$

$$C1$$

RN 885069-43-2 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 885069-44-3 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c} OMe \\ N \\ N \\ N \\ NH-CH_2-CH_2 \\ \hline \\ C1 \\ \end{array}$$

RN 885069-45-4 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \\ \text{N} \\ \text{NH-CH}_2\text{-CH}_2 \\ \end{array}$$

RN 885069-46-5 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \text{N} & \text{N} \\ \text{NH-CH}_2\text{-CH}_2 \\ \end{array}$$

RN 885069-47-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885069-52-3 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} & & \text{NH}_2 \\ \hline & \text{N} & \text{NH} - \text{CH}_2 - \text{CH}_2 \\ \hline \end{array}$$

RN 885069-53-4 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885069-54-5 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885069-55-6 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 885069-56-7 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \hline \\ \text{Ne-S} \\ \hline \\ \text{O} \end{array}$$

RN 885069-57-8 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 885069-60-3 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \\ \text{N} \\ \text{N} \\ \text{NH-CH}_2\text{-CH}_2 \\ \\ \text{C1} \\ \end{array}$$

RN 885069-61-4 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885069-62-5 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & \text{OMe} \\ & \text{Me} \\ \text{Me}_2\text{N}-\text{CH}_2-\text{CH}_2-\text{O}-\text{C}-\text{C} \\ & \text{O} \\ \text{O} \\ \text{Me} \end{array}$$

RN 885069-64-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & \text{OMe} \\ \hline \\ \text{O} \\ \hline \\ \text{MeO-} \text{CH}_2\text{-}\text{C-}\text{NH-}\text{CH}_2\text{-}\text{CH}_2 \\ \hline \end{array}$$

RN 885069-65-8 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \\ \text{NH-CH}_2\text{-CH}_2 \\ \\ \text{F} \end{array}$$

RN 885069-67-0 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$C1$$
 CH_2-CH_2-NH
 HO_2C
 CH_2-CH_2-NH

RN 885069-72-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

● HCl

B85066-06-8P, 3-[2-Methoxy-6-[[2-(4-methoxyphenyl)ethyl]amino]pyri
midin-4-yl]benzenesulfonyl chloride 885066-74-0P,
[2-(3,4-Dimethoxyphenyl)ethyl][6-(3,4-dimethoxyphenyl)-2methylsulfonylpyrimidin-4-yl]amine 885066-77-3P,
[2-Methylsulfonyl-6-(3-methoxyphenyl)pyrimidin-4-yl][2-(4methoxyphenyl)ethyl]amine 885067-30-1P 885067-33-4P
885067-35-6P 885067-53-8P, N-(1-Iminoethyl)-3-[2-methoxy6-[[2-(4-methoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzamide
885067-96-9P, 2-[3-[6-[[2-(2,4-Dichlorophenyl)ethyl]amino]-2methylpyrimidin-4-yl]phenyl]-2-methylpropionitrile 885068-19-9P
885068-25-7P, [3-[6-[[2-(2-Fluoro-4-trifluoromethylphenyl)ethyl]am
ino]-2-methoxypyrimidin-4-yl]phenyl]acetonitrile 885068-26-8P,
[6-[3-(2-Aminoethyl)phenyl]-2-methoxypyrimidin-4-yl][2-(2-fluoro-4-trifluoromethylphenyl)ethyl]amine 885068-30-4P,

3-[6-[[2-(2-Fluoro-4-trifluoromethylphenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]phenol 885068-40-6P, <math>3-[6-[[2-(3,4-

Difluorophenyl)ethyl]amino]-2-methoxypyrimidin-4-yl]phenol

885068-53-1P, 2-[2-Fluoro-5-[2-methoxy-6-[[2-(4-

trifluoromethoxyphenyl)ethyl]amino]pyrimidin-4-yl]phenyl]-2-

methylpropionic acid methyl ester

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of aminopyrimidines as prostaglandin D2 receptor antagonists)

RN 885066-06-8 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 885066-74-0 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 885066-77-3 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

RN 885067-30-1 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & \text{OMe} \\ & \text{NH} \\ & \text{HO-NH-C-CH}_2\text{--}\text{O} \\ & \text{C1} \\ \end{array}$$

RN 885067-33-4 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} & \text{C1} \\ \text{NH} & \text{N} \\ \text{HO-NH-C-CH}_2 & \text{NH-CH}_2\text{-CH}_2 \\ \end{array}$$

RN 885067-35-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & \text{OMe} & & \text{C1} \\ & \text{NH} & & \text{NH} - \text{CH}_2 - \text{CH}_2 \\ & \text{HO-NH-C-CH}_2 - & & \text{F} \end{array}$$

RN 885067-53-8 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & \text{OMe} \\ & \text{N} \\ \text{Me-C-NH-C} \\ & \text{NH} \\ & \text{NH} \end{array} \begin{array}{c} \text{OMe} \\ & \text{NH-CH}_2\text{-CH}_2 \end{array}$$

RN 885067-96-9 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & \text{Me} & \\ & \text{CN} & \text{N} \\ \text{Me} & \text{C} \\ & \text{Me} & \\ & \text{C1} \end{array}$$

RN 885068-19-9 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} & \text{OMe} & \\ \hline & \text{C1} & \\ & \text{CH}_2\text{-}\text{CH}_2\text{-}\text{NH} & \\ \hline & \text{O} & \\ \hline \end{array}$$

RN 885068-25-7 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \\ \text{NC-CH}_2 \end{array} \\ \begin{array}{c} \text{NH-CH}_2\text{-CH}_2 \\ \\ \text{F} \end{array}$$

RN 885068-26-8 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} \\ \\ \text{N} \\ \text{NH-CH}_2\text{-CH}_2 \\ \end{array}$$

RN 885068-30-4 CAPLUS CN INDEX NAME NOT YET ASSIGNED

HO NH-
$$CH_2$$
- CH_2

F

RN 885068-40-6 CAPLUS CN INDEX NAME NOT YET ASSIGNED

RN 885068-53-1 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c} \text{OMe} \\ \text{NC-CH}_2 \\ \text{NC-CH}_2 \\ \end{array}$$

RN 885068-43-9 CAPLUS CN INDEX NAME NOT YET ASSIGNED

$$\begin{array}{c|c} \text{OMe} & \text{F} \\ \text{N} & \text{N} \\ \text{NH-} & \text{CH}_2 - \text{CH}_2 \end{array}$$

RN 885068-89-3 CAPLUS CN INDEX NAME NOT YET ASSIGNED

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ANSWER 4 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
L10
AN
     2006:301346 CAPLUS
DN
     144:350708
     Novel pyrimidine compounds, process for their preparation, pharmaceutical
ΤI
     compositions, and their use as antiinflammatory, cytotoxic, rheumatic,
     immunosuppressive and cardiovascular agents for treatment of diseases
     Kalleda, Srinivas; Padakanti, Srinivas; Kumar Swamy, Nalivela;
IN
     Yeleswarapu, Koteswar Rao; Alexander, Christopher W.; Khanna, Ish Kumar;
     Iqbal, Javed; Pillarisetti, Sivaram; Pal, Manojit; Barange, Deepak
     Reddy US Therapeutics, Inc., USA
PA
SO
     PCT Int. Appl., 336 pp.
     CODEN: PIXXD2
DT
     Patent
     English
LΑ
FAN.CNT 2
                          KIND
                                  DATE
                                               APPLICATION NO.
     PATENT NO.
                                                                        DATE
                                             WO 2005-US34243
                                  20060330
PΙ
     WO 2006034473
                           A2
                                                                        20050923
         W: AE, AG, AL, AM, AT \lambda AU, AZ, \betaA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, PD, II, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ,
             NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG,
              SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN,
             YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
     US 2006084644
                           Α1
                                  20060420
                                               US 2005-234257
                                                                        20050923
     US 2006084645
                            A1
                                  20060420
                                               US 2005-234695
                                                                        20050923
PRAI US 2004-612374P
                                  20040923
                            Ρ
     The invention provides heterocyclic compds., particularly substituted
     pyrimidines of formula I, methods and compns. for making and using these
     heterocyclic compds., and methods for treating a variety of diseases and
     disease states, including atherosclerosis, arthritis, restenosis, diabetic
     nephropathy, or dyslipidemia, or disease states mediated by the low
     expression of Perlecan. Compds. of formula I wherein R1, R2 and R4 are
     independently (un) substituted (hetero) aryl or (un) substituted
     heterocyclyl; and their pharmaceutically acceptable salts, prodrugs,
     diastereoisomeric mixts., enantiomers, tautomers, and racemic mixts.
     thereof are claimed in this invention. Example compound II was prepared by
     acylation of 4-methoxyacetophenone with di-Et carbonate; the resulting Et
     4-methoxybenzoylacetate underwent cyclization with guanidine carbonate to
     give 2-amino-6-(4-methoxyphenyl)pyrimidin-4-ol, which was converted to
     4-chloro-6-(methoxyphenyl)pyrimidin-2-ylamine, which underwent amination
     with 3-chloro-4-methoxyaniline to give compound II. The invention compds.
     were evaluated for their antiinflammatory, proliferative, cardiovascular,
     and immunosuppressive activity (no data).
IT
     881193-27-7P 881194-61-2P 881194-64-5P
     881194-67-8P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (drug candidate; preparation of pyrimidine compds. and their use as
```

antiinflammatory, proliferative, rheumatic, immunosuppressive and

cardiovascular agents for treatment of diseases)

RN 881193-27-7 CAPLUS

CN 2,4-Pyrimidinediamine, N2-(3-chloro-4-methoxyphenyl)-6-phenyl-N4-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 881194-61-2 CAPLUS

CN 4-Pyrimidinamine, 2-(ethylthio)-6-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 881194-64-5 CAPLUS

CN 2(1H)-Pyrimidinone, 4-phenyl-6-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 881194-67-8 CAPLUS

CN 4-Pyrimidinamine, 2-chloro-6-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

```
L10
    ANSWER 5 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
     2006:292375 CAPLUS
AN
DN
     144:350703
     Preparation of 4-aminomethylpyrimidines as ppar-alpha modulators
ΤI
IN
     Dittrich-Wengenroth, Elke; Baerfacker, Lars; Kretschmer, Axel;
     Hirth-Dietrich, Claudia; Ellinghaus, Peter; Raabe, Martin; Bischoff,
     Hilmar; Pilger, Christian; Rosentreter, Ulrich; Bartel, Stephan; Lustig,
     Klemens; Kern, Armin; Lang, Dieter; Bauser, Marcus
PA
     Bayer Healthcare AG, Germany
SO
     PCT Int. Appl., 140 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     German
FAN.CNT 1
     PATENT NO.
                          KIND
                                 DATE
                                             APPLICATION NO.
                                                                      DATE
PΙ
     WO 2006032384
                          A1
                                 20060330
                                             WO 2005-EP9734
                                                                      20050910
         W: AE, AG, AL, AM, \AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
             NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,
             SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,
             ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ,/NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
                                 20060330
                                             DE 2004-102004046623
                                                                      20040925
     DE 102004046623
                          A1
PRAI DE 2004-102004046623 A
                                20040925
     Title compds. I [X = (CH2)\hat{n}; n = 0-2; A = 0, S; Z = (CH2)\hat{m}; O, NR9; m =
     0-2; R9 = H, alkyl; R1 = aryl, 5-t0 10-membered heteroaryl; R2 = H, aryl,
     alkyl, etc.; R3, R4 = H, alkyl, alkenyl, etc.; R5, R6 = H, alkyl, alkoxy,
     etc.; R7 = NHR16, OR17; R16 = H, alkyl, alkylsulfonyl; R17 = H,
     O-protecting group with provisos; R8 = H, alkyl; D, E = N, CH with
     provisos] and their pharmaceutically acceptable salts and formulations
     were prepared For example, HCl-mediated deprotection of of t-Bu ester II [Y
     = O-tBu] afforded claimed aminomethylpyrimidine II [Y = OH] in 31% yield.
     In ppar-\alpha receptor EC50 assays, compds. I exhibited values from 1
     \mu M to 1 nM.
IT
     881686-45-9P 881686-46-0P 881686-47-1P
     881686-48-2P 881686-49-3P 881686-50-6P
     881686-51-7P 881686-52-8P 881686-53-9P
     881686-54-0P 881686-55-1P 881686-56-2P
     881686-57-3P 881686-58-4P 881686-59-5P
     881686-64-2P 881686-65-3P 881686-77-7P
     881686-78-8P 881686-79-9P 881687-03-2P
     881687-04-3P 881687-05-4P 881687-06-5P
     881687-07-6P 881687-08-7P 881687-09-8P
     881687-10-1P 881687-11-2P 881687-12-3P
     881687-13-4P 881687-15-6P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (preparation of 4-aminomethylpyrimidines as ppar-alpha modulators)
RN
     881686-45-9 CAPLUS
     Propanoic acid, 2-[[4-[[(2-methoxyethyl)]6-[3-(trifluoromethyl)phenyl]-4-
CN
```

pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, hydrochloride (9CI) (CA INDEX NAME)

●x HCl

RN 881686-46-0 CAPLUS

CN Propanoic acid, 2-[[4-[[[6-(3-chlorophenyl)-4-pyrimidinyl](2-methoxyethyl)amino]methyl]phenyl]thio]-2-methyl-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & \text{CH}_2-\text{CH}_2-\text{OMe} \\ \hline & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

●x HCl

RN 881686-47-1 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-methoxyethyl)[6-(3-methylphenyl)-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & \text{CH}_2\text{--}\text{CH}_2\text{--}\text{OMe} \\ \hline & & & \text{N} & \\ & & & \text{N} & \\ & & & \text{N} & \\ \end{array}$$

RN 881686-48-2 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-methoxyethyl)[6-(4-methylphenyl)-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-(9CI) (CA INDEX NAME)

RN 881686-49-3 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-furanylmethyl)[6-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, hydrochloride (9CI) (CA INDEX NAME)

●x HCl

RN 881686-50-6 CAPLUS

CN Propanoic acid, 2-[[4-[[[6-(3-chlorophenyl)-4-pyrimidinyl](2-furanylmethyl)amino]methyl]phenyl]thio]-2-methyl-, hydrochloride (9CI) (CA INDEX NAME)

$$CH_{2} \longrightarrow CH_{2} \longrightarrow C$$

●x HCl

RN 881686-51-7 CAPLUS

CN Propanoic acid, 2-methyl-2-[[4-[[[6-(3-methylphenyl)-4-pyrimidinyl]amino]methyl]phenyl]thio]-, hydrochloride (9CI) (CA INDEX NAME)

●x HCl

RN 881686-52-8 CAPLUS

CN Propanoic acid, 2-[[4-[[[6-(4-fluoro-3-methylphenyl)-4-pyrimidinyl](2-furanylmethyl)amino]methyl]phenyl]thio]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \text{CH}_2 - N & \text{Me} \\ \hline & CH_2 & \\ & & \\ & \text{Me} & \\ & & \\$$

RN 881686-53-9 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-furanylmethyl)[6-(3-methylphenyl)-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl- (9CI) (CA INDEX NAME)

RN 881686-54-0 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-furanylmethyl)[6-(2-methylphenyl)-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl- (9CI) (CA INDEX NAME)

RN 881686-55-1 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-furanylmethyl)[6-(4-methylphenyl)-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl- (9CI) (CA INDEX NAME)

RN 881686-56-2 CAPLUS

CN Propanoic acid, 2-[[4-[[[6-(2-fluoro-5-methylphenyl)-4-pyrimidinyl](2-methoxyethyl)amino]methyl]phenyl]thio]-2-methyl- (9CI) (CA INDEX NAME)

RN 881686-57-3 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-methoxyethyl)[2-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{F3C} \\ \hline \\ N \\ \hline \\ N \\ \hline \\ N \\ \hline \\ N \\ R \end{array}$$

$$\begin{array}{c} \text{Me} \\ | \\ \text{S-C-CO}_2\text{H} \\ | \\ \text{Me} \end{array}$$

●x HCl

RN 881686-58-4 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-methoxyethyl)[2-(3-methylphenyl)-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, hydrochloride (9CI) (CA INDEX NAME)

Me
$$CH_2-CH_2-OMe$$
 $N-R$

●x HCl

RN 881686-59-5 CAPLUS

CN Propanoic acid, 2-[[4-[[[2-(3-chlorophenyl)-4-pyrimidinyl](2-methoxyethyl)amino]methyl]phenyl]thio]-2-methyl-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Cl} & & \\ & N & \text{N} & \text{CH}_2\text{--}\text{CH}_2\text{--}\text{OMe} \\ & & N & \text{R} \end{array}$$

●x HCl

RN 881686-64-2 CAPLUS

CN Propanoic acid, 2-[[4-[[[6-(3-chlorophenyl)-4-pyrimidinyl]-2-propynylamino]methyl]phenyl]thio]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \\ \text{N} & \text{CH}_2\text{--}\text{C} \\ & \text{CH}_2 \\ & \text{CH}_2 \\ \end{array}$$

RN 881686-65-3 CAPLUS

CN Propanoic acid, 2-methyl-2-[[4-[[(2-thiazolylmethyl)[6-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]- (9CI) (CA INDEX NAME)

RN 881686-77-7 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-methoxyethyl)[6-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \text{CH}_2-\text{CH}_2-\text{OMe} \\ \hline & & & & \\ F_3C & & & & \\ \end{array}$$

RN 881686-78-8 CAPLUS

CN Propanoic acid, 2-[[4-[[[(3,5-dimethyl-4-isoxazolyl)methyl][6-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-(9CI) (CA INDEX NAME)

RN 881686-79-9 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-fluoroethyl)[6-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{N} \\ & \text{N} \\ & \text{N} \\ & \text{CH}_2 - \text{CH}_2 \text{F} \\ & \text{Me} \\ & \text{Me} \\ & \text{Me} \\ \end{array}$$

RN 881687-03-2 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-methoxyethyl)[6-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} F_3C & & CH_2-CH_2-OMe \\ \hline & N & | & | \\ & N-R & \\ \end{array}$$

RN 881687-04-3 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-methoxyethyl)[6-[4-(trifluoromethoxy)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl- (9CI) (CA INDEX NAME)

RN 881687-05-4 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-methoxyethyl)[6-[3-(trifluoromethoxy)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \\ \text{S-C-CO}_2\text{H} \\ \\ \text{Me} \end{array}$$

RN 881687-06-5 CAPLUS

CN Propanoic acid, 2-[[4-[[[6-(4-fluoro-3-methylphenyl)-4-pyrimidinyl](2-methoxyethyl)amino]methyl]phenyl]thio]-2-methyl- (9CI) (CA INDEX NAME)

RN 881687-07-6 CAPLUS

CN Propanoic acid, 2-methyl-2-[[4-[[[(2-methyl-4-thiazolyl)methyl][6-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]- (9CI)

(CA INDEX NAME)

Me
$$CH_2$$
 CH_2 CH_2 CH_2 CH_2 CF_3 CF_3

RN 881687-08-7 CAPLUS

CN Propanoic acid, 2-methyl-2-[[4-[[[(2-methyl-4-thiazolyl)methyl][6-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]- (9CI) (CA INDEX NAME)

RN 881687-09-8 CAPLUS

CN Propanoic acid, 2-methyl-2-[[4-[[[(1-methyl-1H-imidazol-2-yl)methyl][6-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]- (9CI) (CA INDEX NAME)

RN 881687-10-1 CAPLUS

CN Propanoic acid, 2-methyl-2-[[4-[[[(1-methyl-1H-imidazol-2-yl)methyl][6-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]- (9CI) (CA INDEX NAME)

RN 881687-11-2 CAPLUS

CN Propanoic acid, 2-[[4-[[[(2,4-dimethyl-5-thiazolyl)methyl][6-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-(9CI) (CA INDEX NAME)

$$Me$$
 S
 CH_2
 $N-CH_2$
 Me
 Me
 Me
 S
 S
 S
 Me
 Me
 Me
 Me
 Me

RN 881687-12-3 CAPLUS

CN Propanoic acid, 2-[[4-[[(2,4-dimethyl-5-thiazolyl)methyl][6-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \text{Me} \\ & \text{S} & \text{Me} \\ & \text{S} & \text{C} & \text{CO}_2\text{H} \\ & \text{N} & \text{CH}_2 & \text{Me} \\ & & \text{N} & \text{N} & \text{Me} \\ & & \text{N} & \text{N} & \text{Me} \\ & & \text{N} & \text{N} & \text{N} \\ & & \text{N} & \text{N} \\ & & \text{N} & \text{N} & \text{N} \\ & & \text{N} &$$

RN 881687-13-4 CAPLUS

CN Propanoic acid, 2-[[4-[[[(2,4-dimethyl-5-thiazolyl)methyl][6-(4-methylphenyl)-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl- (9CI) (CA INDEX NAME)

RN 881687-15-6 CAPLUS

CN Propanoic acid, 2-[[4-[[(cyclopropylmethyl)[6-[3-(trifluoromethyl)phenyl]-

4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl- (9CI) (CA INDEX NAME)

IT 881687-25-8P 881687-26-9P 881687-27-0P 881687-28-1P 881687-29-2P 881687-30-5P 881687-31-6P 881687-32-7P 881687-33-8P 881687-34-9P 881687-35-0P 881687-36-1P 881687-38-3P 881687-39-4P 881687-40-7P 881687-45-2P 881687-49-6P 881687-67-8P 881687-68-9P 881687-69-0P 881687-97-4P 881687-99-6P 881688-01-3P 881688-03-5P 881688-05-7P 881688-06-8P 881688-07-9P 881688-08-0P 881688-09-1P 881688-10-4P 881688-11-5P 881688-12-6P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(preparation of 4-aminomethylpyrimidines as ppar-alpha modulators) 881687-25-8 CAPLUS Propanoic acid, 2-[[4-[[(2-methoxyethyl)[6-[3-(trifluoromethyl)phenyl]-4pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester

(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & \text{CH}_2-\text{CH}_2-\text{OMe} \\ \hline & & \text{N} & & \\ \hline & & \text{N} & & \\ \hline & & \text{N} & & \\ \hline & & & \text{R} \end{array}$$

(Reactant or reagent)

RN

CN

$$\begin{array}{c|c} \text{Me O} \\ | & || \\ \text{S-C-C-OBu-t} \\ \\ \text{Me} \end{array}$$

RN 881687-26-9 CAPLUS

Propanoic acid, 2-[[4-[[[6-(3-chlorophenyl)-4-pyrimidinyl](2-CN methoxyethyl)amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & \text{CH}_2-\text{CH}_2-\text{OMe} \\ \hline & & & \\ \text{Cl} & & & \\ \end{array}$$

RN 881687-27-0 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-methoxyethyl)]6-(3-methylphenyl)-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N & CH_2-CH_2-OMe \\ \hline & N & R \\ \end{array}$$

$$\begin{array}{c|c} \text{Me O} \\ & \parallel \\ \text{S-C-C-OBu-t} \\ \\ \text{R-CH}_2 \end{array}$$

RN 881687-28-1 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-methoxyethyl)[6-(4-methylphenyl)-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881687-29-2 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-furanylmethyl)[6-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester

(9CI) (CA INDEX NAME)

RN 881687-30-5 CAPLUS

CN Propanoic acid, 2-[[4-[[[6-(3-chlorophenyl)-4-pyrimidinyl](2-furanylmethyl)amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881687-31-6 CAPLUS

CN Propanoic acid, 2-methyl-2-[[4-[[[6-(3-methylphenyl)-4-pyrimidinyl]amino]methyl]phenyl]thio]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881687-32-7 CAPLUS

CN Propanoic acid, 2-[[4-[[[6-(4-fluoro-3-methylphenyl)-4-pyrimidinyl](2-furanylmethyl)amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester

(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & &$$

RN 881687-33-8 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-furanylmethyl)[6-(3-methylphenyl)-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881687-34-9 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-furanylmethyl)[6-(2-methylphenyl)-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881687-35-0 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-furanylmethyl)[6-(4-methylphenyl)-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881687-36-1 CAPLUS

CN Propanoic acid, 2-[[4-[[[6-(2-fluoro-5-methylphenyl)-4-pyrimidinyl](2-methoxyethyl)amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Me
$$N - CH_2 - CH_2 - OMe$$
 $N - R$

RN 881687-38-3 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-methoxyethyl)[2-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} F_3C \\ \hline \\ N \\ \hline \\ N \\ \hline \\ N \\ \hline \\ N \\ R \end{array}$$

RN 881687-39-4 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-methoxyethyl)[2-(3-methylphenyl)-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881687-40-7 CAPLUS

CN Propanoic acid, 2-[[4-[[[2-(3-chlorophenyl)-4-pyrimidinyl](2-methoxyethyl)amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881687-45-2 CAPLUS

CN Propanoic acid, 2-[[4-[[[6-(3-chlorophenyl)-4-pyrimidinyl]-2-propynylamino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881687-49-6 CAPLUS

CN Propanoic acid, 2-methyl-2-[[4-[[(2-thiazolylmethyl)[6-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881687-67-8 CAPLUS

CN Propanoic acid, 2-[[4-[[[(3,5-dimethyl-4-isoxazolyl)methyl][6-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881687-68-9 CAPLUS

CN Propanoic acid, 2-methyl-2-[[4-[[[6-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881687-69-0 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-fluoroethyl)[6-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881687-97-4 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-methoxyethyl)[6-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881687-99-6 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-methoxyethyl)[6-[4-(trifluoromethoxy)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881688-01-3 CAPLUS

CN Propanoic acid, 2-[[4-[[(2-methoxyethyl)[6-[3-(trifluoromethoxy)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester

(9CI) (CA INDEX NAME)

RN 881688-03-5 CAPLUS

CN Propanoic acid, 2-[[4-[[[6-(4-fluoro-3-methylphenyl)-4-pyrimidinyl](2-methoxyethyl)amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881688-05-7 CAPLUS

CN Propanoic acid, 2-methyl-2-[[4-[[[(2-methyl-4-thiazolyl)methyl][6-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881688-06-8 CAPLUS

CN Propanoic acid, 2-methyl-2-[[4-[[[(2-methyl-4-thiazolyl)methyl][6-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881688-07-9 CAPLUS

CN Propanoic acid, 2-methyl-2-[[4-[[[(1-methyl-1H-imidazol-2-yl)methyl][6-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881688-08-0 CAPLUS

CN Propanoic acid, 2-methyl-2-[[4-[[[(1-methyl-1H-imidazol-2-yl)methyl][6-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881688-09-1 CAPLUS

CN Propanoic acid, 2-[[4-[[[(2,4-dimethyl-5-thiazolyl)methyl]]6-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Me & N & Me \\ \hline S & Me & O \\ \hline CH_2 & S-C-C-OBu-t \\ \hline N-CH_2 & Me \\ \end{array}$$

RN 881688-10-4 CAPLUS

CN Propanoic acid, 2-[[4-[[[(2,4-dimethyl-5-thiazolyl)methyl][6-[3-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881688-11-5 CAPLUS

CN Propanoic acid, 2-[[4-[[[(2,4-dimethyl-5-thiazolyl)methyl][6-(4-methylphenyl)-4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 881688-12-6 CAPLUS

CN Propanoic acid, 2-[[4-[[(cyclopropylmethyl)[6-[3-(trifluoromethyl)phenyl]-

4-pyrimidinyl]amino]methyl]phenyl]thio]-2-methyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L10
     ANSWER 6 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
     2006:269060 CAPLUS
AN
DN
     144:311786
TΙ
     Substituted aniline derivatives as KCNQ subtype potassium ion channel
     openers, their preparation, pharmaceutical compositions, and use in
IN
     Tornoee, Christian Wenzel; Rottlaender, Mario; Greve, Daniel Rodriguez;
     Khanzhin, Nikolay; Ritzen, Andreas; Watson, William Patrick
PA
     H. Lundbeck A/S, Den.
SO
     PCT Int. Appl., 101 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                          KIND
                                  ĎATE
                                              APPLICATION NO.
                                                                       DATE
                                              WO 2005-DK560
                               / 20060323
ΡI
     WO 2006029623
                           A1
                                                                       20050902
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, MM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
             NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,
             SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,
             ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MG, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ/NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
                                  20040913
PRAI DK 2004-1394
                           Α
     US 2004-609856P
                           P
                                  20040913
OS
     MARPAT 144:311786
     The invention relates to aniline derivs. of formula I, which are openers
AB
     of the KCNQ family of potassium ion channels. In compds. I, Z is O or S;
     q is 0 or 1; R1 and R2 are independently selected from halo, cyano, amino,
     C1-6 alkyl, C2-6 alkenyl, C3-8 cycloalkyl, C3-8 heterocyclyl, aryl,
     heteroaryl, etc.; R3 is selected from C1-8 alkyl, C2-8 alkenyl, C3-8
     cycloalkyl, aryl-C1-6 alkyl, aryl-C3-8 cycloalkyl, C3-8 heterocyclyl-C1-6
     alkyl, heteroaryl-C1-6 alkyl, etc.; and R4 is selected from halo, cyano,
     C1-6 alkyl, C2-6 alkenyl, C3-8 cycloalkyl, C3-8 heterocyclyl, aryl,
     heteroaryl, aryl-C1-6 alkyl, (un) substituted amino, etc. The invention
     also relates to the preparation of I, pharmaceutical compns. comprising a
     compound I with one or more pharmaceutically acceptable carriers or
     diluents, as well as to the use of the compns. for the treatment of a
     disorder or disease being responsive to an increased ion flow in a
     potassium channel, such as epilepsy. Amidation of cyclopentaneacetyl
     chloride with 4-bromo-2,6-dimethylaniline gave acetamide II, which
     underwent substitution with pyrrole to give acetanilide III. Some compds.
     of the invention express EC50 values below 200 nM in an assay for affinity
     for the KCNQ2 receptor subtype.
     879648-61-0P, [2,6-Dimethyl-4-[(4-methyl-2-phenylpyrimidin-5-
IΤ
     ylmethyl)amino]phenyl]carbamic acid propyl ester
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (drug candidate; preparation of aniline derivs. as openers of KCNQ family
        potassium ion channels)
```

879648-61-0 CAPLUS

RN

CN Carbamic acid, [2,6-dimethyl-4-[[(4-methyl-2-phenyl-5-pyrimidinyl)methyl]amino]phenyl]-, propyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} & \text{Me} \\ & \text{O} & \\ & \text{NH-CH}_2 & \text{N} \\ & \text{NN-PrO-C-NH} & \\ & \text{NN-Ph} \end{array}$$

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 7 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
ΑN
     2006:232088 CAPLUS
DN
     144:312100
     Preparation of substituted pyridines and pyrimidines as vanilloid receptor
TI
     Norman, Mark H.; Pettus, Liping H.; Wang, Xianghong; Zhu, Jiawang
IN
PA
     U.S. Pat. Appl. Publ., 96 pp.
SO
     CODEN: USXXCO
DT
     Patent
LΑ
     English
FAN.CNT 1
                          KIND
                                 ĎΑΤΕ
                                              APPLICATION NO.
                                                                      DATE
     PATENT NO.
                                 20060316
                                              US 2005-226844
                                                                      20050913
PI
     US 2006058308
                           A1
                                              WO 2005-US32660
     WO 2006031852
                           A1
                                 20060323
                                                                      20050913
         W: AE, AG, AL, AM, AT, AU, AZ,
                                          ∕BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
             NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,
             SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,
             ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
                                 20040913/
PRAI US 2004-609718P
                           Р
OS
     MARPAT 144:312100
     Title compds. I [J = NH, O \circ r - S; X = N \text{ or } CR2; Y = N \text{ or } CR2, \text{ wherein at}
AB
     least one of X and Y = N; R1 = (un) saturated or partially saturated 5-7
     monocyclic or 6-11 membered bicyclic ring containing 0-4 heteroatoms, wherein
     the available carbon atoms are substituted by 0-2 oxo or thioxo groups,
     the ring may contain addnl. substituents; R2 = halo, (un) substituted
     alkyl, benzyl, etc.; R3 = CN, alkoxy, (un) substituted alkyl, etc.; R4 =
     6-11 membered bicyclic ring containing 0-4 atoms selected from N, O and S,
     wherein the available carbon atoms are substituted by 0-2 oxo or thioxo
     groups, the ring may contain addnl. substituents], and their
     pharmaceutically acceptable salts, are prepared and disclosed as vanilloid
     receptor ligands. Thus, e.g., II was prepared by coupling of
     4-tert-butylphenylboronic acid with 2,4,6-trichloropyrimidine followed by
     subsequent substitutions with 1,4-benzodioxane-6-amine and
     4-methylpiperazine. Selected compds. of the invention exhibited IC50
     values of less than 10 nM in the human VR1 capsaicin antagonist assay.
     should prove useful in treating pain and inflammatory conditions.
IT
     879603-63-1P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of substituted pyridines and pyrimidines as vanilloid receptor
        ligands)
     879603-63-1
RN
                  CAPLUS
CN
     Methanesulfonamide, N-[3-[[[4-[(3-amino-1,2-dihydro-2-oxo-5-
     quinoxalinyl)oxy]-6-[4-(trifluoromethyl)phenyl]-2-
     pyrimidinyl]amino]methyl]phenyl]- (9CI) (CA INDEX NAME)
```

10/671,070

- L10 ANSWER 8 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2006:188882 CAPLUS
- DN 144:432768
- ΤI Optimization of 2,4-diaminopyrimidines as GHS-R antagonists: Side chain exploration
- AU Liu, Bo; Liu, Mei; Xin, Zhili; Zhao, Hongyu; Serby, Michael D.; Kosogof, Christi; Nelson, Lissa T. J.; Szczepankiewicz, Bruce G.; Kaszubska, Wiweka; Schaefer, Verlyn G.; Falls, H. Douglas; Lin, Chun Wel; Collins,
- Christine A.; Sham, Hing L.; Liu, Gang
 Metabolic Disease Research, Global Pharmaceutical Research and CS Development, Abbott Laboratories, Abbott Park, IL, 60064-6098, USA Bioorganic & Medicinal Chemistry Letters (2006), 16(7), 1864-1868
- SO CODEN: BMCLE8; ISSN: 0960-894X
- PB Elsevier B.V.
- DT Journal
- English LΑ
- OS CASREACT 144:432768
- AB The synthesis and structure-activity relationships of the 4- and 6-substituents of 2,4-diaminopyrimidine-based growth hormone secretagogue receptor (GHS-R) antagonists are described. Diaminopyrimidines I [R = 2-norbornenyl, 2-tetrahydrofuranyl] exhibit potent GHS-R antagonism and good selectivity (.apprx.1000-fold) against dihydrofolate reductase.
- IT861102-94-5P 861102-96-7P 885040-55-1P 885040-56-2P 885040-68-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of (methanesulfonylbenzyl)aminophenyl diaminopyrimidines as growth hormone secretagogue receptor antagonists)

RN 861102-94-5 CAPLUS

CN 2,4-Pyrimidinediamine, 6-[(methylphenylamino)methyl]-5-[4-[[[4-(methylsulfonyl)phenyl]methyl]amino]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & &$$

861102-96-7 CAPLUS RN

2,4-Pyrimidinediamine, 5-[4-[[[4-(methylsulfonyl)phenyl]methyl]amino]pheny CN 1]-6-[(phenylamino)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

RN 885040-55-1 CAPLUS

CN 2,4-Pyrimidinediamine, 6-[[(4-fluorophenyl)amino]methyl]-5-[4-[[[4-(methylsulfonyl)phenyl]methyl]amino]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} R & & O \\ \hline NH-CH_2 & & O \\ \hline S-Me \\ O & & O \\ \end{array}$$

RN 885040-56-2 CAPLUS

CN 2,4-Pyrimidinediamine, 6-[[(4-fluorophenyl)methylamino]methyl]-5-[4-[[[4-(methylsulfonyl)phenyl]methyl]amino]phenyl]- (9CI) (CA INDEX NAME)

RN 885040-68-6 CAPLUS

CN 2,4-Pyrimidinediamine, 6-ethyl-5-[4-[[[4-(methylsulfonyl)phenyl]methyl]ami no]phenyl]-N4-(phenylmethyl)- (9CI) (CA INDEX NAME)

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/671,070

L10 ANSWER 9 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

2006:111075 CAPLUS AN

DN 144:246539

Parallel synthesis of 5-cyano-6-aryl-2-thiouracil derivatives as ΤI inhibitors for hepatitis C viral NS5B RNA-dependent RNA polymerase

Ding, Yili; Girardet, Jean-Luc; Smith, Kenneth L.; Larson, Gary; Prigaro, Brett; Wu, Jim Z.; Yao, Nanhua Valeant Pharmaceuticals International, Costa Mesa, CA, 92626, USA Bioorganic Chemistry (2006), 34(1), 26-38 CODEN: BOCMBM; ISSN: 0045-2068 ΑU

CS

SO

PΒ Elsevier

DTJournal

LA English

From random screening of our compound libraries, we identified a hit compound AΒ (I) with an IC50 of 27 μM against hepatitis C viral NS5B RNA-dependent RNA polymerase. By using a parallel synthetic strategy, a series of its derivs. were synthesized. From their anti-HCV activity screening, compds. with single digital 3.8 micromolar activity were obtained.

ΙT 877460-76-9P 877460-78-1P 877460-81-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(cyano aryl thiouracil derivs. as inhibitors for hepatitis C viral NS5B RNA-dependent RNA polymerase)

RN877460-76-9 CAPLUS

5-Pyrimidinecarbonitrile, 4-(4-bromophenyl)-6-[[2-(3-CN methoxyphenyl)ethyl]amino]-2-[[[2-(trifluoromethyl)phenyl]methyl]thio]-(9CI) (CA INDEX NAME)

$$F_{3}C$$

$$CH_{2}$$

$$S$$

$$S$$

$$N$$

$$N$$

$$N$$

$$CH_{2}-CH_{2}-NH$$

$$CN$$

RN 877460-78-1 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-(4-bromophenyl)-6-[(2-phenylethyl)amino]-2-[[[2-(trifluoromethyl)phenyl]methyl]thio]- (9CI) (CA INDEX NAME)

$$F_{3}C$$

$$CH_{2}$$

$$S$$

$$N$$

$$N$$

$$N$$

$$E$$

$$CN$$

$$Br$$

$$CN$$

RN 877460-81-6 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-(4-bromophenyl)-6-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-2-[[[2-(trifluoromethyl)phenyl]methyl]thio]-(9CI) (CA INDEX NAME)

$$F_3C$$

$$CH_2$$

$$S$$

$$OMe$$

$$OMe$$

$$OMe$$

$$CN$$

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/671,070

L10 ANSWER 10 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2006:38998 CAPLUS

DN 144:292704

TI A Highly Regioselective Amination of 6-Aryl-2,4-dichloropyrimidine

AU Peng, Zhi-Hui; Jøurnet, Michel; Humphrey, Guy

CS Department of Process Research, Merck & Co., Inc., Rahway, NJ, 07065, USA

SO Organic Letters (2006), 8(3), 395-398 CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society

DT Journal

LA English

OS CASREACT 144:292704

AB A highly regioselective amination of 6-aryl-2,4-dichloropyrimidines with aliphatic secondary amines and aromatic amines which strongly favors the formation of the C4-substituted product has been developed. The reactions with aliphatic amines are carried out using LiHMDS as the base and are catalyzed by Pd, while the aromatic amines require no catalyst.

IT 878199-61-2P 878199-62-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(regioselective amination of 6-aryl-2,4-dichloropyrimidines)

RN 878199-61-2 CAPLUS

CN 4-Pyrimidinamine, 2-chloro-6-(4-fluorophenyl)-N-methyl-N-(phenylmethyl)-(9CI) (CA INDEX NAME)

RN 878199-62-3 CAPLUS

CN 2-Pyrimidinamine, 4-chloro-6-(4-fluorophenyl)-N-methyl-N-(phenylmethyl)-(9CI) (CA INDEX NAME)

RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L10 ANSWER 11 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2005:1346218 CAPLUS
- DN 144:88321
- TI Preparation of triazinyl and other carboxamides as inhibitors of histone deacetylase
- IN Delorme, Daniel; Woo, Soon Hyung; Vaisburg, Arkadii; Moradei, Oscar; Leit, Silvana; Raeppel, Stephane; Frechette, Sylvie; Bouchain, Giliane
- PA Methylgene, Inc., Can.
- SO U.S. Pat. Appl. Publ., 324 pp., Cont.-in-part of U.S. Ser. No. 358,556. CODEN: USXXCO
- DT Patent
- LA English
- FAN.CNT 3

1111.011 3						
		PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	PI	US 2005288282	A 1	20051229	US 2005-91025	20050325
		US 2004106599	A 1	20040603	US 2002-242304	20020912
		US 2004142953	A1	20040722	US 2003-358556	20030204
		US 6897220	B2	20050524		
		JP 2005255683	A2	20050922	JP 2005-80310	20050318
	PRAI	US 2001-322402P	P	20010914		
		US 2002-391728P	P	20020626		
		US 2002-242304	A2	20020912		
		US 2003-358556	A2	20030204		
		JP 2003-528544	A3	20020912		
	OC	MADDAM 144.00221				

OS MARPAT 144:88321

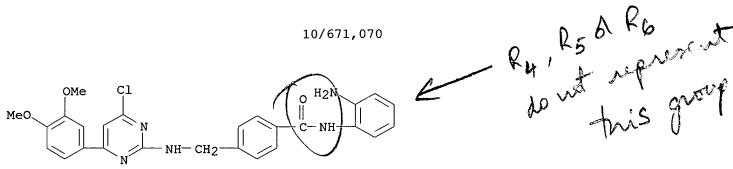
AΒ The invention provides compds. and methods for inhibiting histone deacetylase enzymic activity. Such compds. include carboxamides I [Cy2 = (un) substituted cycloalkyl, aryl, heteroaryl, heterocyclyl (each of which is optionally fused to one or two aryl or heteroaryl rings, or to one or two (un)saturated cycloalkyl or heterocyclic rings); X1 = a bond, M1L2M1, L2M2L2 (wherein L2 = a bond, alkylene, alkenylene, alkynylene; M1 = O, S, SO, NHCO, etc.; M2 = M1, heteroarylene, heterocyclylene); Ar2 = (un) substituted (hetero) arylene; R5, R6 = H, alkyl, aryl, aralkyl; q = 0-1; Ay2 = (un)substituted 5-6 membered cycloalkkyl, heterocyclyl or heteroaryl substituted with an amino or hydroxy moiety; with provisos] which were prepared and claimed. E.g., a multi-step synthesis of II, starting from Me 4-(aminomethyl)benzoate. HCl, was given. The invention also provides compns. and methods for treating cell proliferative diseases and conditions. Antineoplastic effects of some I are illustrated for colorectal, pulmonary and pancreatic neoplasms; also the combined antineoplastic effect of histone deacetylase inhibitors and histone deacetylase antisense oligonucleotides on tumor cells in vivo was demonstrated. Although the methods of preparation are not claimed, hundreds of example prepns. are included.

IT 503043-79-6P 503043-80-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of triazinyl and other carboxamides as inhibitors of histone deacetylase for treating cell proliferative disorders)

- RN 503043-79-6 CAPLUS
- CN Benzamide, N-(2-aminophenyl)-4-[[[4-chloro-6-(3,4-dimethoxyphenyl)-2-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)



503043-80-9 CAPLUS RN

CN Benzamide, N-(2-aminophenyl)-4-[[[4-(3,4-dimethoxyphenyl)-2pyrimidinyl]amino]methyl]- (9CI) (CA-INDEX NAME)

MeO NH-
$$CH_2$$
 $C-NH$

```
L10
     ANSWER 12 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2005:1331285 CAPLUS
DN
     144:69847
TI
     Preparation of 4-phenylpyridine-2-carbonitrile derivs. as inhibitors of
     cathepsin K and cathepsin S
     Cai, Jiaqiang; Rankovic, Zoran; Moir, Jennifer Helen
IN
PA
     Akzo Nobel N.V., Neth.
SO
     PCT Int. Appl., 71 pp.
     CODEN: PIXXD2
DT
     Patent
LА
     English
FAN.CNT 1
                          KIND
                                  DATE!
     PATENT NO.
                                              APPLICATION NO.
                                                                       DATE
                                              ______
PΙ
     WO 2005121106
                           Α1
                                  20051222
                                              WO 2005-EP6266
                                                                       20050609
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
             LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
             NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,
             SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,
             ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
             RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
             MR, NE, SN, TD,
PRAI EP 2004-253491
                           Α
                                  20040611
     EP 2004-106949
                                  20041223
OS
     MARPAT 144:69847
AB
     Title compds. I [wherein R (one to three) = (un)substituted alkyl, alkoxy,
     cyano, etc.; R1 = H or alkyl; R2 = (un)substituted alkyl, alkoxy, aryloxy,
     etc., and pharmaceutically acceptable salts thereof] were prepared as
     inhibitors of cathepsin K and cathepsin S. For instance,
     3'-trifluoromethylacetophenone underwent successive condensation with Et
     butyrate (76%), cyclization with urea in the presence of HCl (72%),
     chlorination with POCl3 (100%) and substitution with CuCN (8%) to give II.
     I showed inhibition of human cathepsin K with pIC50 > 6 (pIC50 > 7 for
           Therefore, I and their pharmaceutical compns. are useful for the
     treatment of cathepsin K and cathepsin S related diseases, such as
     atherosclerosis, bone diseases, inflammation, immune disorders and pain.
     871793-50-9P, 4-(3-Phenylaminopropyl)-6-(3-
IT
     trifluoromethylphenyl)pyrimidine-2-carbonitrile
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (inhibitor; preparation of phenylpyridinecarbonitrile derivs. as inhibitors
        of cathepsin K and cathepsin S)
RN
     871793-50-9 CAPLUS
CN
     2-Pyrimidinecarbonitrile, 4-[3-(phenylamino)propyl]-6-[3-
     (trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)
```

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L10
     ANSWER 13 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2005:1170507 CAPLUS
DN
     143:440431
ΤI
     Substituted thiazole and pyrimidine derivatives as melanocortin receptor
     modulators
TN
     Mjalli, Adnan M. M.; Gaddam, Bapu R.; Qabaja, Ghassan; Subramanian,
     Govindan; Zhu, Jeff; Dankwardt, John; Arimilli, Murty N.; Andrews, Robert
     C.; Victory, Samuel; Tian, Ye E.
     Transtech Pharma, Inc., USA
PA
     PCT Int. Appl., 179 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
                                  DATE
                           KIND
                                               APPLICATION NO.
                                                                        DATE
     PATENT NO.
                               // 20051103
PΙ
     WO 2005103022
                            A1
                                               WO 2005-US13386
                                                                        20050420
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
              CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
              GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
              NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL,
              SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA,
              ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
             MR, NE, SN, TD, TG
                                  20051124
                                               US 2005-110499
                                                                        20050420
     US 2005261294
                            A1
PRAI US 2004-563882P
                            Ρ
                                  20040420
OS
     MARPAT 143:440431
     Title compds. I [A = substituted amine, substituted alkyl, substituted
AB
     sulfonamide, etc.; m = 0-2; R1 and R2 independently = H, halo, alkyl,
     etc., or R1 and R2 may be taken together to form part of a fused
     carbocyclic ring, aromatic ring, heteroarom. ring, etc.; W = S, N=N, or
     CR3=N; R3 = H, halo, alkyl, etc.], methods of their preparation, pharmaceutical
     compns. comprising the compds. of Formula (I), and methods of use in
     treating human or animal disorders are disclosed. Thus, e.g., II was
     prepared by cyclocondensation of 2-bromo-1(4-isopropylphenyl)ethanone
     (preparation given) with thiourea followed by reaction with
     chlorosulfonyl-acetic acid tert-Bu ester (preparation given). I showed an
     increase in cAMP production and a reduction in fluorescence polarization in
assays
     and possess an effective concentration for half maximal effect (EC50) in the
     assay of less than 14 \mu M. The compds. of the invention can be useful
     as inhibitors of action of AgRP on a melanocortin receptor and thus can be
     useful for the management, treatment, control, or the adjunct treatment of
     diseases which may be responsive to the modulation of melanocortin
     receptors including obesity-related disorders.
ΙT
     868590-55-0P 868590-72-1P 868590-73-2P
     868590-74-3P 868590-75-4P 868590-76-5P
     868590-77-6P 868590-78-7P 868590-79-8P
     868590-80-1P 868590-81-2P 868590-82-3P
     868590-83-4P 868590-84-5P 868590-85-6P
     868590-86-7P 868590-87-8P 868590-88-9P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
```

(Uses)

(preparation of thiazole and pyrimidine derivs. as melanocortin receptor modulators)

RN 868590-55-0 CAPLUS

CN Glycine, N-[(4-chlorophenyl)methyl]-N-[2-[4-(1-methylethyl)phenyl]-4-pyrimidinyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 868590-72-1 CAPLUS

CN Benzoic acid, 3-[[cyclopentyl[4-[4-[(cis-4-methylcyclohexyl)oxy]phenyl]-2-pyrimidinyl]amino]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 868590-73-2 CAPLUS

CN Benzoic acid, 3-[[2-[4-(cyclohexylmethoxy)phenyl]-4pyrimidinyl]cyclopentylamino]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

RN 868590-74-3 CAPLUS

CN Benzoic acid, 4-[[[2-[4-(1-methylethyl)phenyl]-4-pyrimidinyl](2-thienylmethyl)amino]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 868590-75-4 CAPLUS

CN Benzoic acid, 2-[[[4-[4-(1-methylethyl)phenyl]-2-pyrimidinyl](2-thienylmethyl)amino]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

RN 868590-76-5 CAPLUS

CN Benzoic acid, 3-[[[4-[4-(1-methylethyl)phenyl]-2-pyrimidinyl](2-thienylmethyl)amino]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 868590-77-6 CAPLUS

CN Benzoic acid, 2-[[[4-[4-(1-methylethoxy)phenyl]-2-pyrimidinyl](2-thienylmethyl)amino]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

RN 868590-78-7 CAPLUS

CN Benzoic acid, 2-[[(2-thienylmethyl)[4-[4-(trifluoromethoxy)phenyl]-2-pyrimidinyl]amino]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 868590-79-8 CAPLUS

CN Benzoic acid, 2-[[[4-(4-phenoxyphenyl)-2-pyrimidinyl](2-thienylmethyl)amino]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 868590-80-1 CAPLUS

CN Benzoic acid, 2-[[[4-(4-methoxyphenyl)-2-pyrimidinyl](2-thienylmethyl)amino]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 868590-81-2 CAPLUS

CN Benzoic acid, 2-[[[4-(4-fluorophenyl)-2-pyrimidinyl](2-thienylmethyl)amino]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} S & CH_2-N & N \\ \hline \\ HO_2C & \end{array}$$

● HCl

RN 868590-82-3 CAPLUS

CN Benzoic acid, 3-[[cyclopentyl[4-[4-[(trans-4-methylcyclohexyl)oxy]phenyl]-2-pyrimidinyl]amino]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 868590-83-4 CAPLUS

CN Benzoic acid, 4-[[[4-[4-(1-methylethyl)phenyl]-2-pyrimidinyl](2-thienylmethyl)amino]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 868590-84-5 CAPLUS

CN Benzoic acid, 2-[[[2-[4-(1-methylethyl)phenyl]-4-pyrimidinyl](2-thienylmethyl)amino]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 868590-85-6 CAPLUS

CN Benzoic acid, 3-[[[2-[4-(1-methylethyl)phenyl]-4-pyrimidinyl](2-thienylmethyl)amino]methyl]-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 868590-86-7 CAPLUS

CN Benzoic acid, 2-[[[2-[4-(phenylmethoxy)phenyl]-4-pyrimidinyl](2-thienylmethyl)amino]methyl]-, sodium salt (9CI) (CA INDEX NAME)

Na

RN 868590-87-8 CAPLUS

CN Benzoic acid, 3-[[[2-[4-(phenylmethoxy)phenyl]-4-pyrimidinyl](2-thienylmethyl)amino]methyl]-, sodium salt (9CI) (CA INDEX NAME)

Na

RN 868590-88-9 CAPLUS

CN Benzoic acid, 4-[[[2-[4-(phenylmethoxy)phenyl]-4-pyrimidinyl](2-thienylmethyl)amino]methyl]-, sodium salt (9CI) (CA INDEX NAME)

Na

RN 868591-61-1 CAPLUS
CN Benzoic acid, 3-[[cyclopentyl[4-(4-hydroxyphenyl)-2-pyrimidinyl]amino]methyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 868591-62-2 CAPLUS

CN Benzoic acid, 3-[[cyclopentyl[4-[4-[(cis-4-methylcyclohexyl)oxy]phenyl]-2-pyrimidinyl]amino]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 868591-64-4 CAPLUS

CN Benzoic acid, 3-[[cyclopentyl[2-[4-(phenylmethoxy)phenyl]-4-pyrimidinyl]amino]methyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 868591-65-5 CAPLUS

CN Benzoic acid, 3-[[cyclopentyl[2-(4-hydroxyphenyl)-4-pyrimidinyl]amino]methyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 868591-66-6 CAPLUS

CN Benzoic acid, 3-[[[2-[4-(cyclohexylmethoxy)phenyl]-4-pyrimidinyl]cyclopentylamino]methyl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ \parallel & \\ \hline \\ CH_2 & \\ \hline \\ N & \\ \end{array}$$

RN 868591-67-7 CAPLUS

CN Benzoic acid, 4-[[[2-[4-(1-methylethyl)phenyl]-4-pyrimidinyl](2-thienylmethyl)amino]methyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 868591-68-8 CAPLUS

CN Benzoic acid, 3-[[cyclopentyl[4-[4-[(trans-4-methylcyclohexyl)oxy]phenyl]-2-pyrimidinyl]amino]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN

868591-69-9 CAPLUS
Benzoic acid, 4-[[[4-[4-(1-methylethyl)phenyl]-2-pyrimidinyl](2-thienylmethyl)amino]methyl]-, methyl ester (9CI) (CA INDEX NAME) CN

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L10
     ANSWER 14 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2005:1075803 CAPLUS
DN
     143:367317
ΤI
     Preparation of N-(2-amino and 2-hydroxy) phenyl carboxamides as inhibitors
     of histone deacetylase
     Delorme, Daniel; Vaisburg, Arkadii; Moradei, Oscar; Leit, Silvana;
TN
     Raeppel, Stephane; Frechette, Sylvie; Bouchain, Giliane; Zhou, Zhihong;
     Paquin, Isabelle; Gaudette, Frederic; Isakovic, Ljubomir
     Methylgene Inc., Can.
PA
     PCT Int. Appl., 245 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LА
     English
FAN.CNT 1
                          KIND
                                 ÓATE
                                             APPLICATION NO.
                                                                     DATE
     PATENT NO.
PΙ
     WO 2005092899
                          A1.
                                 20051006
                                             WO 2005-CA454
                                                                     20050329
         W: AE, AG, AL, AM, AT
                                 AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM,
             SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM,
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
             MR, NE, SN, TD, TG
                                 20051103
                                             US 2005-90713
                                                                     20050325
     US 2005245518
                          A1
PRAI US 2004-556828P
                           Ρ
                                 20040326
     US 2005-90713
                                 20050325
                           Α
     WO 2005-IB802
                           Α
                                 20050325
     MARPAT 143:367317
OS
     The invention relates to N-(2-amino and 2-hydroxy) phenyl carboxamides
AΒ
     (2-TC6H4NHC(O)(CH:CH)qAr-X-Cy(I); variables defined below; e.g.
     (E) - N - (2 - Aminophenyl) - 3 - [4 - [(2 - hydroxyethyl)] - (1 + indol - 3 - 1)]
     yl)ethyl]amino]methyl]phenyl]acrylamide (shown as II)) useful for
     inhibiting histone deacetylase (HDAC) enzymic activity. The invention
     also provides a method for inhibiting histone deacetylase in a cell using
     said compds. as well as a method for treating cell proliferative diseases
     and conditions using said HDAC inhibitors. Further, the invention
     provides pharmaceutical compns. comprising the HDAC inhibiting compds. and
     a pharmaceutically acceptable carrier. For I: Cy is aryl, heteroaryl,
     cycloalkyl, or heterocyclyl, each of which is (un) substituted and each of
     which is optionally fused to ≥1 aryl or heteroaryl rings, or to
     ≥1 saturated or partially unsatd. cycloalkyl or heterocyclic rings,
     each of which rings is (un)substituted; X = a chemical bond, L, W-L, L-W, and
     L-W-L, wherein W, at each occurrence, is S, O, C:O, or N(R9), where R9 =
     H, alkyl, hydroxyalkyl, and tert-butoxycarbonyl; and L = C1-C4 alkylene;
     Ar is arylene or heteroarylene, each of which is (un)substituted; q = 0-1;
     and T is NH2 or OH, provided that when Cy is naphthyl, X is -CH2-, Ar is
     Ph, and q = 0-1, T is not OH. Although the methods of preparation are not
     claimed, 215 example prepns. and/or characterization data are included.
     For example, II was prepared in 6 steps (59, 83, 97, 79, 96 and 80 % yields)
     starting from (E)-4-formylcinnamic acid and involving intermediates Me
     (E)-3-(4-formylphenyl) acrylate, Me (E)-3-[4-[[[2-(1H-indol-3-
     yl)ethyl]amino]methyl]phenyl]acrylate, Me (E)-3-[4-[[[2-[(tert-
     butyldimethylsilanyl)oxy]ethyl][2-(1H-indol-3-
```

```
yl)ethyl]amino]methyl]phenyl]acrylate, (E)-3-[4-[[[2-[(tert-
         butyldimethylsilanyl)oxy]ethyl][2-(1H-indol-3-
         yl)ethyl]amino]methyl]phenyl]acrylic acid and (E)-N-(2-aminophenyl)-3-[4-
          [[[2-[(tert-butyldimethylsilanyl)oxy]ethyl][2-(1H-indol-3-
         yl)ethyl]amino]methyl]phenyl]acrylamide.
         866000-02-4P, N-(2-Aminophenyl)-4-[[[4-(4-methoxyphenyl)pyrimidin-
         2-yl]amino]methyl]benzamide 866000-03-5P, 4-[[[4-(3-
         Acetylphenyl)pyrimidin-2-yl]amino]methyl]-N-(2-aminophenyl)benzamide
         866000-04-6P, N-(2-Aminophenyl)-4-[[[4-(3,4-
         difluorophenyl)pyrimidin-2-yl]amino]methyl]benzamide 866000-05-7P
          , N-(2-Aminophenyl)-4-[[[4-(3-trifluoromethoxyphenyl)pyrimidin-2-
         yl]amino]methyl]benzamide 866000-07-9P, N-(2-Aminophenyl)-4-[[[4-
          (3,4,5-trimethoxyphenyl)pyrimidin-2-yl]amino]methyl]benzamide
         866000-08-0P, N-(2-Aminophenyl)-4-[[[4-(3-fluoro-4-
         methoxyphenyl)pyrimidin-2-yl]amino]methyl]benzamide 866000-09-1P
          , N-(2-Aminopheny1)-4-[[[4-[4-[2-(morpholin-4-y1)ethoxy]pheny1]pyrimidin-2-
         yl]amino]methyl]benzamide 866000-13-7P,
         N-(2-Aminophenyl)-4-[[[4-[3-(2-dimethylaminoethoxy)phenyl]pyrimidin-2-
         yl]amino]methyl]benzamide hydrochloride 866000-14-8P,
         N-(2-Aminopheny1)-4-[[[4-[3-[2-(morpholin-4-y1)ethoxy]pheny1]pyrimidin-2-
         yl]amino]methyl]benzamide 866000-15-9p, N-(2-Aminophenyl)-4-[[[4-
          [4-(2-dimethylaminoethoxy)phenyl]pyrimidin-2-yl]amino]methyl]benzamide
         866000-31-9P, N-(2-Aminophenyl)-4-[[[4-(4-(2-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethoxy)-4-(3-dimethylaminoethylami
         3-fluorophenyl]pyrimidin-2-yl]amino]methyl]benzamide 866000-35-3P
          , N-(2-Aminophenyl)-4-[[[4-[4-[(morpholin-4-yl)methyl]phenyl]pyrimidin-2-
         yl]amino]methyl]benzamide hydrochloride
         RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
          (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
                (drug candidate; preparation of N-(2-amino and 2-hydroxy)phenyl carboxamides
               as inhibitors of histone deacetylase)
RN
          866000-02-4 CAPLUS
          Benzamide, N-(2-aminophenyl)-4-[[[4-(4-methoxyphenyl)-2-
CN
         pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)
```

$$\begin{array}{c|c} \text{MeO} & \text{O} & \text{H}_2\text{N} \\ \hline & \text{N} & \text{NH-CH}_2 \\ \hline \end{array}$$

RN 866000-03-5 CAPLUS
CN Benzamide, 4-[[[4-(3-acetylphenyl)-2-pyrimidinyl]amino]methyl]-N-(2-aminophenyl)- (9CI) (CA INDEX NAME)

RN 866000-04-6 CAPLUS

CN Benzamide, N-(2-aminophenyl)-4-[[[4-(3,4-difluorophenyl)-2-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)

RN 866000-05-7 CAPLUS

CN Benzamide, N-(2-aminophenyl)-4-[[[4-[3-(trifluoromethoxy)phenyl]-2-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)

RN 866000-07-9 CAPLUS

CN Benzamide, N-(2-aminophenyl)-4-[[[4-(3,4,5-trimethoxyphenyl)-2-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)

RN 866000-08-0 CAPLUS

CN Benzamide, N-(2-aminophenyl)-4-[[[4-(3-fluoro-4-methoxyphenyl)-2-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)

MeO
$$N$$
 $NH-CH_2$ $C-NH$

RN 866000-09-1 CAPLUS

CN Benzamide, N-(2-aminophenyl)-4-[[[4-[4-[2-(4-morpholinyl)ethoxy]phenyl]-2-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)

RN 866000-13-7 CAPLUS

CN Benzamide, N-(2-aminophenyl)-4-[[[4-[3-[2-(dimethylamino)ethoxy]phenyl]-2-pyrimidinyl]amino]methyl]-, hydrochloride (9CI) (CA INDEX NAME)

●x HCl

RN 866000-14-8 CAPLUS

CN Benzamide, N-(2-aminophenyl)-4-[[[4-[3-[2-(4-morpholinyl)ethoxy]phenyl]-2-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)

RN 866000-15-9 CAPLUS

CN Benzamide, N-(2-aminophenyl)-4-[[[4-[4-[2-(dimethylamino)ethoxy]phenyl]-2-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)

RN 866000-31-9 CAPLUS

CN Benzamide, N-(2-aminophenyl)-4-[[[4-[4-[2-(dimethylamino)ethoxy]-3-fluorophenyl]-2-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)

$$Me_2N-CH_2-CH_2-O$$

$$N$$

$$N$$

$$NH-CH_2$$

RN 866000-35-3 CAPLUS

CN Benzamide, N-(2-aminophenyl)-4-[[[4-[4-(4-morpholinylmethyl)phenyl]-2-pyrimidinyl]amino]methyl]-, hydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & O \\
 & N \\
 & O \\
 & N \\
 & O \\$$

•x HCl

CN Benzoic acid, 4-[[[4-[4-[2-(4-morpholinyl)ethoxy]phenyl]-2-pyrimidinyl]amino]methyl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ \parallel \\ CH_2-NH \\ \hline \\ N \\ \end{array}$$

RN 866000-12-6 CAPLUS

CN Benzoic acid, 4-[[[4-[4-[2-(4-morpholinyl)ethoxy]phenyl]-2-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)

$$CH_2-NH$$
 $O-CH_2-CH_2-NH$

RN 866000-33-1 CAPLUS
CN Benzoic acid, 4-[[[4-(3-fluoro-4-hydroxyphenyl)-2-pyrimidinyl]amino]methyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 866000-34-2 CAPLUS

CN Benzoic acid, 4-[[[4-[4-[2-(dimethylamino)ethoxy]-3-fluorophenyl]-2-pyrimidinyl]amino]methyl]-, methyl ester (9CI) (CA INDEX NAME)

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L10
     ANSWER 15 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
ΑN
     2005:823690 CAPLUS
DN
     143:229874
     Preparation of pyrimidine derivatives as orexin receptors antagonists
TI
     Aranyi, Peter; Balogh, Maria; Batori, Sandor; Bence, Judit; Finet, Michel;
TN
     Kapui, Zoltan; Philippo, Christophe; Szabo, Tibor; Szlavik, Zoltan;
     Toemoeskoezi, Zsuzsanna; Urban-Szabo, Katalin; Venier, Olivier
PA
     Sanofi-Aventis, Fr.
SO
     PCT Int. Appl., 104 pp.
     CODEN: PIXXD2
DT
     Patent
LА
     English
FAN.CNT 1
                          KIND
                                             APPLICATION NO.
                                                                      DATE
     PATENT NO.
                                 DATE
                                 20050818
PΙ
     WO 2005075458
                          · A1
                                             WO 2005-HU10
                                                                      20050208
     WO 2005075458
                           C1
                                \20060119
         W: AE, AG, AL, AM, AT, AU, AZ,
                                         BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW,
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
             MR, NE, SN, TD, TG
                                 20040210
PRAI HU 2004-405
                           Α
OS
     MARPAT 143:229874
     The title compds. I [Ar = Ph or a 5-6 membered heterocyclic ring containing
AB
     1-3 identical or different heteroatoms or methylenedioxyphenyl group
     (these groups may optionally be substituted with one or more identical or
     different alkyl group, halo, hydroxy, alkoxy, trihalomethyl, NHalkyl,
     N(alkyl) or NHC(O) alkyl group); X = alkyl, (un) substituted NH2,
     alkylthio, etc.; R, Y, W = H, alkyl; Z = OH, halo, alkoxy, etc.; or R + Y
     may represent II (together with the included N and C atoms; wherein A =
     CH2, O, NH, N(alkyl); n = 0-2); or R + Z together may represent a (CH2)mG
     (m = 1-3; G = O, CH2, NH, N(alkyl)); Z + W together may represent an oxo
     group; Q = (un) substituted Ph or 5-6 membered heterocyclic ring containing 1-3
     heteroatoms], useful as orexin receptor antagonists which are selective to
     orexin I receptors, were prepared Thus, reacting 2-dimethylamino-4-
     phenylpyrimidine-5-carboxylic acid with L-phenylephrine hydrochloride
     afforded L-I (Ar = Ph; X = NMe2; R = Me; Y, W = H; Z = OH; Z = OH
     3-(HO)C6H4]. The compds. I exhibit IC50 values of < 1000 nM with the
     preferred compds. I having IC50 of < 100 nM (specific IC50 values against
     Orexin-1 and Orexin-2 were given for six representative compds. I).
     pharmaceutical composition comprising the compound I is disclosed.
IT
     862837-38-5P
     RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (preparation of pyrimidine derivs. as orexin receptors antagonists)
RN
     862837-38-5 CAPLUS
CN
     2-Piperidinemethanol, \alpha-(3-methoxyphenyl)-1-[[2-
     [methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]-,
     (\alpha R, 2R) - rel - (9CI) (CA INDEX NAME)
```

Relative stereochemistry.

IT 862836-09-7P 862836-10-0P 862836-11-1P 862836-12-2P 862836-13-3P 862836-14-4P 862836-15-5P 862836-19-9P 862836-20-2P 862836-23-5P 862836-25-7P 862836-54-2P 862836-56-4P 862836-65-5P 862836-66-6P 862836-67-7P 862836-72-4P 862837-06-7P 862837-07-8P 862837-08-9P 862837-09-0P 862837-10-3P 862837-11-4P 862837-12-5P 862837-13-6P 862837-14-7P 862837-16-9P 862837-17-0P 862837-19-2P 862837-20-5P 862837-21-6P 862837-37-4P 862837-39-6P 862837-40-9P 862837-41-0P 862837-42-1P 862837-43-2P 862837-44-3P 862837-45-4P 862837-46-5P 862837-48-7P 862837-49-8P 862837-50-1P 862837-51-2P 862837-52-3P 862837-53-4P 862837-54-5P 862837-55-6P 862837-56-7P 862837-57-8P 862837-58-9P 862837-59-0P 862837-60-3P 862837-62-5P 862837-63-6P 862837-64-7P 862837-66-9P 862837-67-0P 862837-68-1P 862837-69-2P 862837-70-5P 862837-71-6P 862837-72-7P 862837-73-8P 862837-74-9P 862837-75-0P 862837-76-1P 862837-77-2P 862837-78-3P 862837-79-4P 862837-80-7P 862837-81-8P 862837-82-9P 862837-83-0P 862837-84-1P 862837-85-2P 862837-86-3P 862837-87-4P 862837-88-5P 862837-89-6P 862837-90-9P 862837-91-0P 862837-92-1P 862837-93-2P 862837-94-3P 862837-95-4P 862837-96-5P 862837-97-6P 862839-35-8P 862839-37-0P 862839-39-2P 862839-41-6P 862839-50-7P 862839-69-8P 862839-71-2P 862839-73-4P 862839-95-0P 862839-98-3P 862840-00-4P 862840-02-6P 862840-04-8P 862840-06-0P 862840-08-2P 862840-11-7P 862840-13-9P 862840-17-3P 862840-19-5P 862840-21-9P 862840-30-0P 862840-33-3P 862840-39-9P 862840-44-6P 862840-49-1P 862840-54-8P 862840-58-2P 862840-62-8P 862840-66-2P 862840-70-8P 862840-74-2P 862840-78-6P 862840-82-2P 862840-85-5P 862840-91-3P

862840-94-6P 862840-97-9P 862841-00-7P 862841-03-0P 862841-06-3P 862841-09-6P 862841-12-1P 862841-15-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrimidine derivs. as orexin receptors antagonists) 862836-09-7 CAPLUS

RN 862836-09-7 CAPLUS
CN 5-Pyrimidinecarboxamide, N-[2-hydroxy-2-(3-hydroxyphenyl)ethyl]-N-methyl-2[methyl(phenylmethyl)amino]-4-phenyl-, hydrate (2:1) (9CI) (CA INDEX NAME)

●1/2 H₂O

RN 862836-10-0 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-hydroxy-2-(3-hydroxyphenyl)ethyl]-N-methyl-4-phenyl-2-[(phenylmethyl)amino]-, monohydrate (9CI) (CA INDEX NAME)

H20

RN 862836-11-1 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[(2-hydroxyethyl) (phenylmethyl) amino]-N-[2-hydroxy-2-(3-hydroxyphenyl) ethyl]-N-methyl-4-phenyl-, monohydrate (9CI) (CA INDEX NAME)

● H₂O

RN 862836-12-2 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(2-chlorophenyl)-N-[2-hydroxy-2-(3-hydroxyphenyl)ethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-, monohydrate (9CI) (CA INDEX NAME)

● H2O

RN 862836-13-3 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(2-chlorophenyl)-N-[(2S)-2-hydroxy-2-(3-hydroxyphenyl)ethyl]-N-methyl-2-[methyl(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 862836-14-4 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-hydroxy-2-(3-hydroxyphenyl)ethyl]-N-methyl-4-(2-methylphenyl)-2-[methyl(phenylmethyl)amino]-(9CI) (CA INDEX NAME)

HO OH Me O
$$CH-CH_2-N-C$$
 N $N-CH_2-Ph$ Me

RN 862836-15-5 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-hydroxy-2-(3-hydroxyphenyl)ethyl]-4-(2-methoxyphenyl)-N-methyl-2-[methyl(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

HO OH Me O
$$CH-CH_2-N-C$$
 OMe $N-CH_2-Ph$ Me

RN 862836-19-9 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-hydroxy-2-(3-hydroxyphenyl)ethyl]-N-methyl-4-phenyl-2-[(2-phenylethyl)amino]-, monohydrate (9CI) (CA INDEX NAME)

H2O

RN 862836-20-2 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-N-[2-hydroxy-2-(3-hydroxyphenyl)ethyl]-N-methyl-4-phenyl-, dihydrate (9CI) (CA INDEX NAME)

●2 H₂O

RN 862836-23-5 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[(2-chlorophenyl)methyl]amino]-N-[2-hydroxy-2-(3-hydroxyphenyl)ethyl]-N-methyl-4-phenyl-(9CI) (CA INDEX NAME)

HO OH Me O C1 C1
$$CH-CH_2-N-C$$
 N $NH-CH_2$

RN 862836-25-7 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-hydroxy-2-(3-hydroxyphenyl)ethyl]-4-(2-iodophenyl)-N-methyl-2-[methyl(phenylmethyl)amino]-, hydrate (2:1) (9CI) (CA INDEX NAME)

●1/2 H₂O

RN 862836-54-2 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-hydroxy-2-[3-(phenylmethoxy)phenyl]ethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl-, hydrate (5:1) (9CI) (CA INDEX NAME)

●1/5 H₂O

RN 862836-56-4 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(2-chlorophenyl)-N-[2-hydroxy-2-[3-(phenylmethoxy)phenyl]ethyl]-N-methyl-2-[methyl(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 862836-65-5 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[(1R,2S)-2-hydroxy-1-methyl-2-phenylethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl-, hydrate (4:1), rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

●1/4 H₂O

RN 862836-66-6 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(2-chlorophenyl)-N-[(1R,2S)-2-hydroxy-1-methyl-2-phenylethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 862836-67-7 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[(1R,2S)-2-hydroxy-1-methyl-2-phenylethyl]-N-methyl-4-phenyl-2-[(phenylmethyl)amino]-, hydrate (2:1), rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

●1/2 H₂O

RN 862836-72-4 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[(2-chlorophenyl)methyl]amino]-N-[(1R,2S)-2-hydroxy-1-methyl-2-phenylethyl]-N-methyl-4-phenyl-, hydrate (2:1), rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

●1/2 H₂O

RN 862837-06-7 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl-, monohydrate (9CI) (CA INDEX NAME)

● H₂O

RN 862837-07-8 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-hydroxy-2-(2-hydroxyphenyl)ethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl-, hydrate (4:1) (9CI) (CA INDEX NAME)

●1/4 H₂O

RN 862837-08-9 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-hydroxy-2-(2-methoxyphenyl)ethyl]-N-methyl-2-

[methyl(phenylmethyl)amino]-4-phenyl-, hydrate (5:1) (9CI) (CA INDEX NAME)

●1/5 H₂O

RN 862837-09-0 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(3-fluorophenyl)-2-hydroxyethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl- (9CI) (CA INDEX NAME)

RN 862837-10-3 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(4-fluorophenyl)-2-hydroxyethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl-, monohydrate (9CI) (CA INDEX NAME)

● н20

RN 862837-11-4 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-hydroxy-2-(3-methoxyphenyl)ethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl-, monohydrate (9CI) (CA INDEX NAME)

● H2O

RN 862837-12-5 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-hydroxy-2-(4-methoxyphenyl)ethyl]-N-methyl-2[methyl(phenylmethyl)amino]-4-phenyl-, hydrate (4:1) (9CI) (CA INDEX
NAME)

●1/4 H₂O

RN 862837-13-6 CAPLUS

CN 5-Pyrimidinecarboxamide, N-(2-hydroxy-2-phenylethyl)-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl-, monohydrate (9CI) (CA INDEX NAME)

● H2O

RN 862837-14-7 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-hydroxy-2-[3-(1-methylethoxy)phenyl]ethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl-, hydrate (5:1) (9CI) (CA INDEX NAME)

●1/5 H₂O

RN 862837-16-9 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(3-aminophenyl)-2-hydroxyethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl-, hydrate (2:1) (9CI) (CA INDEX NAME)

●1/2 H₂O

RN 862837-17-0 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-[3-[(2,2-dimethyl-1-oxopropyl)amino]phenyl]-2-hydroxyethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl-, monohydrate (9CI) (CA INDEX NAME)

● H₂O

RN 862837-19-2 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(3,4-dihydroxyphenyl)-2-hydroxyethyl]-N-

methyl-4-phenyl-2-[(phenylmethyl)amino]-, monohydrate (9CI) (CA INDEX NAME)

● H2O

RN 862837-20-5 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-hydroxy-2-(3-nitrophenyl)ethyl]-N-methyl-4-phenyl-2-[(phenylmethyl)amino]-, monohydrate (9CI) (CA INDEX NAME)

● H2O

RN 862837-21-6 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(3-aminophenyl)-2-hydroxyethyl]-N-methyl-4-phenyl-2-[(phenylmethyl)amino]-, dihydrochloride, dihydrate (9CI) (CA INDEX NAME)

●2 HCl

●2 H₂O

RN 862837-37-4 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]- α -phenyl-, (α R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 862837-39-6 CAPLUS

CN 2-Piperidinemethanol, α-(3-hydroxyphenyl)-1-[[2-[methyl (phenylmethyl) amino]-4-phenyl-5-pyrimidinyl]carbonyl]-, (αR,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 862837-40-9 CAPLUS

CN 2-Piperidinemethanol, α-(3-fluorophenyl)-1-[[2-[methyl (phenylmethyl) amino]-4-phenyl-5-pyrimidinyl]carbonyl]-, (αR, 2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 862837-41-0 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]- α -3-pyridinyl-, (α R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 862837-42-1 CAPLUS

CN 2-Piperidinemethanol, 1-[[4-(2-chlorophenyl)-2-[methyl(phenylmethyl)amino]-5-pyrimidinyl]carbonyl]-α-phenyl-, (αR,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 862837-43-2 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]- α -2-pyridinyl-, (α R,2S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 862837-44-3 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(2-bromophenyl)-N-[2-(3,4-dichlorophenyl)-2-hydroxyethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-, monohydrate (9CI) (CA INDEX NAME)

C1 OH Me O
$$N-CH_2-Ph$$
 $N-CH_2-Ph$ $N-CH_2-Ph$

● H2O

RN 862837-45-4 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(3,4-dichlorophenyl)-2-hydroxyethyl]-4-(2-fluorophenyl)-N-methyl-2-[methyl(phenylmethyl)amino]-, hydrate (2:1) (9CI) (CA INDEX NAME)

C1 OH Me O
$$CH-CH_2-N-C$$
 N $N-CH_2-Ph$

●1/2 H₂O

RN 862837-46-5 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(2-bromophenyl)-N-[2-(3,4-dihydroxyphenyl)-2-hydroxyethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-, monohydrate (9CI) (CA INDEX NAME)

OH Me O
$$CH-CH_2-N-C$$
 N N-CH2-Ph

● H2O

RN 862837-48-7 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(2-bromophenyl)-N-[2-hydroxy-2-(3-hydroxyphenyl)ethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-, monohydrate (9CI) (CA INDEX NAME)

● H2O

RN 862837-49-8 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(4-chlorophenyl)-2-hydroxyethyl]-4-(2-fluorophenyl)-N-methyl-2-[methyl(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 862837-50-1 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(3-chlorophenyl)-2-hydroxyethyl]-N-methyl-2[methyl(phenylmethyl)amino]-4-phenyl-, hydrate (2:1) (9CI) (CA INDEX
NAME)

●1/2 H₂O

RN 862837-51-2 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(3,4-difluorophenyl)-2-hydroxyethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl-, hydrate (2:1) (9CI) (CA INDEX NAME)

●1/2 H₂O

RN 862837-52-3 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(3-chlorophenyl)-2-hydroxyethyl]-N-methyl-4-phenyl-2-[(phenylmethyl)amino]-, hydrate (2:3) (9CI) (CA INDEX NAME)

●3/2 H₂O

RN 862837-53-4 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(4-chlorophenyl)-2-hydroxyethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl- (9CI) (CA INDEX NAME)

RN 862837-54-5 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(4-cyanophenyl)-2-hydroxyethyl]-N-methyl-4-phenyl-2-[(phenylmethyl)amino]-, monohydrate (9CI) (CA INDEX NAME)

● н20

RN 862837-55-6 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(4-chlorophenyl)-2-hydroxyethyl]-N-methyl-4-phenyl-2-[(phenylmethyl)amino]-, monohydrate (9CI) (CA INDEX NAME)

● H₂O

RN 862837-56-7 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(1,3-benzodioxol-5-yl)-2-hydroxyethyl]-N-methyl-4-phenyl-2-[(phenylmethyl)amino]-, hydrate (2:3) (9CI) (CA INDEX NAME)

●3/2 H₂O

RN 862837-57-8 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(1,3-benzodioxol-5-yl)-2-hydroxyethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl-, monohydrate (9CI) (CA INDEX NAME)

● H₂O

RN 862837-58-9 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(2-chlorophenyl)-N-[2-(4-chlorophenyl)-2-hydroxyethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-, monohydrate (9CI) (CA INDEX NAME)

C1 OH Me O
$$CH-CH_2-N-C$$
 N $N-CH_2-Ph$ Me

● H₂O ·

RN 862837-59-0 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(2-chlorophenyl)-N-[2-(3,4-dihydroxyphenyl)-2-hydroxyethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-, monohydrate (9CI) (CA INDEX NAME)

● H2O

RN 862837-60-3 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(4-cyanophenyl)-2-hydroxyethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl-, hydrate (2:1) (9CI) (CA INDEX NAME)

●1/2 H₂O

RN 862837-62-5 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(2-fluorophenyl)-N-[2-hydroxy-2-(3-hydroxyphenyl)ethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-, monohydrate (9CI) (CA INDEX NAME)

● H2O

RN 862837-63-6 CAPLUS

CN 2-Piperidinemethanol, $\alpha-(4-fluorophenyl)-1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)$

RN 862837-64-7 CAPLUS

CN 2-Piperidinemethanol, α-(4-methylphenyl)-1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)

RN 862837-66-9 CAPLUS

CN 2-Piperidinemethanol, $1-[[2-[[(3-methoxyphenyl)methyl]amino]-4-phenyl-5-pyrimidinyl]carbonyl]-<math>\alpha$ -phenyl- (9CI) (CA INDEX NAME)

RN 862837-67-0 CAPLUS

CN 2-Piperidinemethanol, α -(3-chlorophenyl)-1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]- (9CI) (CA

INDEX NAME)

RN 862837-68-1 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[[(2-methoxyphenyl)methyl]amino]-4-phenyl-5-pyrimidinyl]carbonyl]- α -phenyl- (9CI) (CA INDEX NAME)

RN 862837-69-2 CAPLUS

CN 2-Piperidinemethanol, $1-[[2-[[(4-chlorophenyl)methyl]methylamino]-4-phenyl-5-pyrimidinyl]carbonyl]-<math>\alpha$ -phenyl- (9CI) (CA INDEX NAME)

RN 862837-70-5 CAPLUS

CN 2-Piperidinemethanol, α -(3-methylphenyl)-1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]- (9CI) (CA

INDEX NAME)

RN 862837-71-6 CAPLUS

CN 2-Piperidinemethanol, $1-[[2-[[(2-chlorophenyl)methyl]methylamino]-4-phenyl-5-pyrimidinyl]carbonyl]-<math>\alpha$ -phenyl- (9CI) (CA INDEX NAME)

RN 862837-72-7 CAPLUS

CN 2-Piperidinemethanol, $1-[[2-[[(4-fluorophenyl)methyl]methylamino]-4-phenyl-5-pyrimidinyl]carbonyl]-<math>\alpha$ -phenyl- (9CI) (CA INDEX NAME)

RN 862837-73-8 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[methyl[(4-methylphenyl)methyl]amino]-4-phenyl-5-pyrimidinyl]carbonyl]- α -phenyl- (9CI) (CA INDEX NAME)

RN 862837-74-9 CAPLUS

CN 2-Piperidinemethanol, α -(2-methylphenyl)-1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
Me \\
| \\
N-CH_2-Ph \\
N-CH_2-Ph \\
R \\
Ph
\end{array}$$

RN 862837-75-0 CAPLUS

CN 2-Piperidinemethanol, α-(2-fluorophenyl)-1-[[2-[methyl (phenylmethyl) amino]-4-phenyl-5-pyrimidinyl] carbonyl]- (9CI) (CA INDEX NAME)

RN 862837-76-1 CAPLUS

CN 2-Piperidinemethanol, α -(4-methoxyphenyl)-1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)

RN 862837-77-2 CAPLUS

CN 2-Piperidinemethanol, α -(4-chlorophenyl)-1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)

RN 862837-78-3 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[[(4-fluorophenyl)methyl]amino]-4-phenyl-5-pyrimidinyl]carbonyl]- α -phenyl- (9CI) (CA INDEX NAME)

RN 862837-79-4 CAPLUS

CN 2-Piperidinemethanol, $1-[[2-[[(4-chlorophenyl)methyl]amino]-4-phenyl-5-pyrimidinyl]carbonyl]-<math>\alpha$ -phenyl- (9CI) (CA INDEX NAME)

RN 862837-80-7 CAPLUS

CN 2-Piperidinemethanol, α -(3-chloro-4-fluorophenyl)-1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)

RN 862837-81-8 CAPLUS

CN 2-Piperidinemethanol, α -(3,4-difluorophenyl)-1-[[2- [methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]- (9CI) (CA

INDEX NAME)

RN 862837-82-9 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[[(3-chlorophenyl)methyl]amino]-4-phenyl-5-pyrimidinyl]carbonyl]- α -phenyl- (9CI) (CA INDEX NAME)

RN 862837-83-0 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[[(4-methoxyphenyl)methyl]methylamino]-4-phenyl-5-pyrimidinyl]carbonyl]-α-phenyl- (9CI) (CA INDEX NAME)

RN 862837-84-1 CAPLUS

CN 2-Piperidinemethanol, α-(4-chloro-3-fluorophenyl)-1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)

RN 862837-85-2 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[[(4-methoxyphenyl)methyl]amino]-4-phenyl-5-pyrimidinyl]carbonyl]-α-phenyl- (9CI) (CA INDEX NAME)

RN 862837-86-3 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]-α-4-pyridinyl- (9CI) (CA INDEX NAME)

RN 862837-87-4 CAPLUS

CN 2-Piperidinemethanol, 1-[[4-(2-fluorophenyl)-2-[methyl(phenylmethyl)amino]-

5-pyrimidinyl]carbonyl] $-\alpha$ -phenyl- (9CI) (CA INDEX NAME)

RN 862837-88-5 CAPLUS

CN 2-Piperidinemethanol, $1-[[2-[[(3-chlorophenyl)methyl]methylamino]-4-phenyl-5-pyrimidinyl]carbonyl]-<math>\alpha$ -phenyl- (9CI) (CA INDEX NAME)

RN 862837-89-6 CAPLUS

CN 2-Piperidinemethanol, α -(2-chlorophenyl)-1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]- (9CI) (CA INDEX NAME)

RN 862837-90-9 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[methyl (phenylmethyl) amino]-4-phenyl-5-pyrimidinyl]carbonyl]- α -3-thienyl- (9CI) (CA INDEX NAME)

RN 862837-91-0 CAPLUS

CN 2-Piperidinemethanol, $1-[[2-[[(3-chloro-4-fluorophenyl)methyl]amino]-4-phenyl-5-pyrimidinyl]carbonyl]-<math>\alpha$ -phenyl- (9CI) (CA INDEX NAME)

RN 862837-92-1 CAPLUS

CN 2-Piperidinemethanol, $1-[[2-[[(3-chloro-4-fluorophenyl)methyl]methylamino]-4-phenyl-5-pyrimidinyl]carbonyl]-<math>\alpha$ -phenyl- (9CI) (CA INDEX NAME)

RN 862837-93-2 CAPLUS

CN 2-Piperidinemethanol, $1-[[4-(4-chlorophenyl)-2-[methyl(phenylmethyl)amino]-5-pyrimidinyl]carbonyl]-<math>\alpha$ -phenyl- (9CI) (CA INDEX NAME)

RN 862837-94-3 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[[(4-chlorophenyl)methyl]amino]-4-(2-fluorophenyl)-5-pyrimidinyl]carbonyl]- α -(3,4-difluorophenyl)- (9CI) (CA INDEX NAME)

RN 862837-95-4 CAPLUS

CN 2-Piperidinemethanol, $1-[[4-(2-chlorophenyl)-2-[[(4-chlorophenyl)methyl]amino]-5-pyrimidinyl]carbonyl]-<math>\alpha$ -(3,4-

difluorophenyl) - (9CI) (CA INDEX NAME)

RN 862837-96-5 CAPLUS

CN 2-Piperidinemethanol, $1-[[2-[[(4-\text{chlorophenyl})\text{methyl}]\text{methylamino}]-4-(2-\text{fluorophenyl})-5-pyrimidinyl]carbonyl]-<math>\alpha$ -(3,4-difluorophenyl)- (9CI) (CA INDEX NAME)

RN 862837-97-6 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[[(3-chloro-4-fluorophenyl)methyl]amino]-4-phenyl-5-pyrimidinyl]carbonyl]-α-3-thienyl- (9CI) (CA INDEX NAME)

RN 862839-35-8 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-hydroxy-2-(3-hydroxyphenyl)ethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl- (9CI) (CA INDEX NAME)

RN 862839-37-0 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-hydroxy-2-(3-hydroxyphenyl)ethyl]-N-methyl-4-phenyl-2-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 862839-39-2 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[(2-hydroxyethyl)(phenylmethyl)amino]-N-[2-hydroxy-2-(3-hydroxyphenyl)ethyl]-N-methyl-4-phenyl- (9CI) (CA INDEX NAME)

RN 862839-41-6 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(2-chlorophenyl)-N-[2-hydroxy-2-(3-hydroxyphenyl)ethyl]-N-methyl-2-[methyl(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 862839-50-7 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-hydroxy-2-(3-hydroxyphenyl)ethyl]-4-(2-iodophenyl)-N-methyl-2-[methyl(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 862839-69-8 CAPLUS

CN 5-Pyrimidinecarboxamide, N-(2-hydroxy-1-methyl-2-phenylethyl)-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl- (9CI) (CA INDEX NAME)

RN 862839-71-2 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(2-chlorophenyl)-N-(2-hydroxy-1-methyl-2-phenylethyl)-N-methyl-2-[methyl(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 862839-73-4 CAPLUS

CN 5-Pyrimidinecarboxamide, N-(2-hydroxy-1-methyl-2-phenylethyl)-N-methyl-4-phenyl-2-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 862839-95-0 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-hydroxy-2-(4-hydroxyphenyl)ethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl- (9CI) (CA INDEX NAME)

RN 862839-98-3 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(4-fluorophenyl)-2-hydroxyethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl- (9CI) (CA INDEX NAME)

RN 862840-00-4 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-hydroxy-2-(3-methoxyphenyl)ethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl- (9CI) (CA INDEX NAME)

RN 862840-02-6 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-hydroxy-2-(4-methoxyphenyl)ethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl- (9CI) (CA INDEX NAME)

RN 862840-04-8 CAPLUS

CN 5-Pyrimidinecarboxamide, N-(2-hydroxy-2-phenylethyl)-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl- (9CI) (CA INDEX NAME)

RN 862840-06-0 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(3-aminophenyl)-2-hydroxyethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl- (9CI) (CA INDEX NAME)

RN 862840-08-2 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(3,4-dihydroxyphenyl)-2-hydroxyethyl]-N-methyl-4-phenyl-2-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 862840-11-7 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(2-bromophenyl)-N-[2-(3,4-dihydroxyphenyl)-2-hydroxyethyl]-N-methyl-2-[methyl(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 862840-13-9 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(2-bromophenyl)-N-[2-hydroxy-2-(3-hydroxyphenyl)ethyl]-N-methyl-2-[methyl(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 862840-17-3 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(1,3-benzodioxol-5-yl)-2-hydroxyethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl- (9CI) (CA INDEX NAME)

RN 862840-19-5 CAPLUS

CN 5-Pyrimidinecarboxamide, 4-(2-chlorophenyl)-N-[2-(3,4-dihydroxyphenyl)-2-hydroxyethyl]-N-methyl-2-[methyl(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

HO OH Me O
$$CH-CH_2-N-C$$
 N $N-CH_2-Ph$ Me

RN 862840-21-9 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[2-(4-cyanophenyl)-2-hydroxyethyl]-N-methyl-2-[methyl(phenylmethyl)amino]-4-phenyl- (9CI) (CA INDEX NAME)

RN 862840-30-0 CAPLUS

CN 2-Piperidinemethanol, α-(4-fluorophenyl)-1-[[2[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]-,
(αR,2R)-rel- (9CI) (CA INDEX NAME)

RN 862840-33-3 CAPLUS

CN 2-Piperidinemethanol, α -(4-methylphenyl)-1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]-, $(\alpha R, 2R)$ -rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 862840-39-9 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[[(3-methoxyphenyl)methyl]amino]-4-phenyl-5-pyrimidinyl]carbonyl]- α -phenyl-, (α R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 862840-44-6 CAPLUS

CN 2-Piperidinemethanol, α-(3-chlorophenyl)-1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]-, (αR,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 862840-49-1 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[[(4-chlorophenyl)methyl]methylamino]-4-phenyl-5-pyrimidinyl]carbonyl]- α -phenyl-, (α R, 2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 862840-54-8 CAPLUS

CN 2-Piperidinemethanol, α-(3-methylphenyl)-1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]-, (αR,2R)-rel- (9CI) (CA INDEX NAME)

RN 862840-58-2 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[[(4-fluorophenyl)methyl]methylamino]-4-phenyl-5-pyrimidinyl]carbonyl]- α -phenyl-, (α R, 2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 862840-62-8 CAPLUS CN 2-Piperidinemethanol, α -(2-methylphenyl)-1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]-, $(\alpha R, 2R)$ -rel- (9CI) (CA INDEX NAME)

RN 862840-66-2 CAPLUS CN 2-Piperidinemethanol, α -(2-fluorophenyl)-1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]-, $(\alpha R, 2R)$ -rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 862840-70-8 CAPLUS
CN 2-Piperidinemethanol, α-(4-methoxyphenyl)-1-[[2[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]-,
 (αR, 2R)-rel- (9CI) (CA INDEX NAME)

RN 862840-74-2 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[[(4-fluorophenyl)methyl]amino]-4-phenyl-5-pyrimidinyl]carbonyl]- α -phenyl-, (α R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 862840-78-6 CAPLUS

CN 2-Piperidinemethanol, α-(3-chloro-4-fluorophenyl)-1-[[2-[methyl (phenylmethyl) amino]-4-phenyl-5-pyrimidinyl]carbonyl]-, (αR,2R)-rel- (9CI) (CA INDEX NAME)

RN 862840-82-2 CAPLUS CN 2-Piperidinemethanol, α -(3,4-difluorophenyl)-1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]-, $(\alpha R, 2R)$ -rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 862840-85-5 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[[(3-chlorophenyl)methyl]amino]-4-phenyl-5-pyrimidinyl]carbonyl]- α -phenyl-, (α R,2R)-rel- (9CI) (CA INDEX NAME)

RN 862840-91-3 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]- α -4-pyridinyl-, (α R,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 862840-94-6 CAPLUS

CN 2-Piperidinemethanol, 1-[[4-(2-fluorophenyl)-2-[methyl(phenylmethyl)amino]-5-pyrimidinyl]carbonyl]- α -phenyl-, (α R, 2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 862840-97-9 CAPLUS

CN 2-Piperidinemethanol, $1-[[2-[[(3-chlorophenyl)methyl]methylamino]-4-phenyl-5-pyrimidinyl]carbonyl]-<math>\alpha$ -phenyl-, $(\alpha R, 2R)$ -rel- (9CI) (CA

INDEX NAME)

Relative stereochemistry.

RN 862841-00-7 CAPLUS

CN 2-Piperidinemethanol, α-(2-chlorophenyl)-1-[[2[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]-,
(αR,2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 862841-03-0 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[methyl(phenylmethyl)amino]-4-phenyl-5-pyrimidinyl]carbonyl]- α -3-thienyl-, (α R,2R)-rel- (9CI) (CA INDEX NAME)

RN 862841-06-3 CAPLUS
CN 2-Piperidinemethanol, 1-[[2-[[(3-chloro-4-fluorophenyl)methyl]amino]-4 phenyl-5-pyrimidinyl]carbonyl]-α-phenyl-, (αR,2R)-rel- (9CI)
 (CA INDEX NAME)

Relative stereochemistry.

RN 862841-12-1 CAPLUS

CN 2-Piperidinemethanol, $1-[[4-(4-chlorophenyl)-2-[methyl(phenylmethyl)amino]-5-pyrimidinyl]carbonyl]-<math>\alpha$ -phenyl-, (α R, 2R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 862841-15-4 CAPLUS

CN 2-Piperidinemethanol, 1-[[2-[[(3-chloro-4-fluorophenyl)methyl]amino]-4-phenyl-5-pyrimidinyl]carbonyl]-α-3-thienyl-, (αR,2R)-rel-(9CI) (CA INDEX NAME)

RN 862838-06-0 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 2-[methyl(phenylmethyl)amino]-4-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 862838-07-1 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 2-[methyl(phenylmethyl)amino]-4-phenyl- (9CI) (CA INDEX NAME)

RN 862838-12-8 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(2-chlorophenyl)-2[methyl(phenylmethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 862838-15-1 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-phenyl-2-[(phenylmethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 862838-16-2 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 2-[(2-hydroxyethyl)(phenylmethyl)amino]-4-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

Eto-C
$$\stackrel{\text{Ph}}{\underset{\text{N}}{|}}$$
 $\stackrel{\text{N-CH}_2-\text{CH}_2-\text{OH}}{\underset{\text{CH}_2-\text{Ph}}{|}}$

RN 862838-18-4 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 2-[[(2-chlorophenyl)methyl]amino]-4-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

Eto-C
$$N$$
 $NH-CH_2$

RN 862838-25-3 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-phenyl-2-[(2-phenylethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

Eto-C
$$N$$
 $NH-CH_2-CH_2-Ph$

RN 862838-26-4 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 2-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-4-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OMe} & \text{OMe} \\ \hline \\ \text{EtO-C} & \text{N} \\ \hline \\ \text{Ph} & \text{NH-CH}_2\text{-CH}_2 \\ \hline \end{array}$$

RN 862838-31-1 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(2-iodophenyl)-2[methyl(phenylmethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 862838-39-9 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-phenyl-2-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 862838-40-2 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 2-[(2-hydroxyethyl)(phenylmethyl)amino]-4-phenyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} \\ & & \\ & & \\ N \\ & & \\ N \\ & \text{CH}_2\text{--} \text{CH}_2\text{--} \text{OH} \\ & \\ & & \\ \text{CH}_2\text{--} \text{Ph} \end{array}$$

RN 862838-41-3 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(2-methylphenyl)-2-[methyl(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 862838-42-4 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(2-methoxyphenyl)-2-[methyl(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 862838-44-6 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 2-[[(2-chlorophenyl)methyl]methylamino]-4-phenyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Me \\ \hline \\ CH_2-N \\ \hline \\ N \\ \hline \\ Ph \\ \end{array}$$

RN 862838-60-6 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-phenyl-2-[(2-phenylethyl)amino]- (9CI) (CA INDEX NAME)

$$HO_2C$$
 N
 $NH-CH_2-CH_2-Ph$

RN 862838-62-8 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 2-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-4-phenyl- (9CI) (CA INDEX NAME)

HO₂C
$$\sim$$
 N \sim NH- CH₂- CH₂ \sim OMe

RN 862838-99-1 CAPLUS

5-Pyrimidinecarboxylic acid, 4-(2-iodophenyl)-2-[methyl(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

CN

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L10 ANSWER 16 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
AN
    2005:698362 CAPLUS
     143:172891
DN
TI
     Preparation of diaminopyrimidines as growth hormone secretagogue receptor
     (GHS-R) antagonists
IN
     Kosogof, Christi; Liu, Bo; Liu, Gang; Liu, Mei; Nelson, Lissa T. J.;
     Serby, Michael D.; Sham, Hing L.; Szczepankiewicz, Bruce G.; Xin, Zhili;
     Zhao, Hongyu
PA
    USA
    U.S. Pat. Appl. Publ., 63 pp.
SO
     CODEN: USXXCO
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     Patent
LΑ
    English
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                                DATE
     PATENT NO.
                                            APPLICATION NO.
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                                            US 2004-947823
                                                                   20040923
    US 2005171131
    US 2005171132
                          Α1
                                20050804
                                            US 2004-948042
                                                                   20040923
PRAI US 2003-506663P
                                20030926
                          Ρ
    MARPAT 143:172891
os
    Title compds. I [A = (hetero)ary1, heterocycle; R2 = alkenyl,
AΒ
    alkenyloxyalkyl, alkoxy, alkoxyalkoxy, etc.; R = H, alkenyl, alkenyloxy,
    etc.; n = 1-4; X = 0, amino, CH2NH; R3 = H, alkenyl, alkoxy, etc.] are
    prepared For instance, 5-[4-[(4-chlorobenzyl)amino]phenyl]-6-
     ethylpyrimidine-2,4-diamine is prepared in 4 steps from 4-
    nitrophenylacetonitrile, propionyl chloride, guanidine hydrochloride and
     4-chlorobenzaldehyde. Compds. of the present invention are found to
     antagonize the function of ghrelin in a range of 0.001 \mu M to about 0.1
    μM and inhibit dihydrofolate reductase in a range of about 0.0001 μM
    to about 0.1 µM. I are useful in the treatment of disorders regulated
    by the action of ghrelin receptor, including Prader-Willi syndrome, eating
    disorder, weight gain, weight-loss maintenance following diet and exercise,
    obesity, and disorders associated with obesity such as noninsulin dependent
    diabetes mellitus.
ΙT
     861102-94-5P, 6-[[Methyl(phenyl)amino]methyl]-5-[4-[[4-
     (methanesulfonyl)benzyl]amino]phenyl]pyrimidine-2,4-diamine
     861102-96-7P, 6-(Anilinomethyl)-5-[4-[[4-
     (methanesulfonyl)benzyl]amino]phenyl]pyrimidine-2,4-diamine
     861103-06-2P, 6-[[(2,3-Dimethoxyphenyl)amino]methyl]-5-[4-[[4-
     (methanesulfonyl)benzyl]amino]phenyl]pyrimidine-2,4-diamine
     861103-36-8P 861103-55-1P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of diaminopyrimidines as growth hormone secretagogue receptor
        (GHS-R) antagonists)
RN
     861102-94-5 CAPLUS
     2,4-Pyrimidinediamine, 6-[(methylphenylamino)methyl]-5-[4-[[[4-
CN
```

(methylsulfonyl)phenyl]methyl]amino]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

RN 861102-96-7 CAPLUS

CN 2,4-Pyrimidinediamine, 5-[4-[[[4-(methylsulfonyl)phenyl]methyl]amino]phenyl]-6-[(phenylamino)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

RN 861103-06-2 CAPLUS

CN 2,4-Pyrimidinediamine, 6-[[(2,3-dimethoxyphenyl)amino]methyl]-5-[4-[[[4-(methylsulfonyl)phenyl]methyl]amino]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OMe} \\ \text{N} \\ \text{N} \\ \text{N} \\ \text{NH}_2 \end{array}$$

RN 861103-36-8 CAPLUS

CN 2,4,6-Pyrimidinetriamine, 5-[4-[[[4-(methylsulfonyl)phenyl]methyl]amino]phenyl]-N4-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph-CH}_2-\text{NH} & \text{N} & \text{NH}_2 \\ \hline \\ \text{O} & & & & & \\ \text{Me-S} & & & & \\ \text{O} & & & & \\ \end{array}$$

RN 861103-55-1 CAPLUS

CN 2,4,6-Pyrimidinetriamine, 5-[4-[[[4-(methylsulfonyl)phenyl]methyl]amino]phenyl]-N4-(2-phenylethyl)- (9CI) (CA INDEX NAME)

IT 861103-38-0P, N'-Benzyl-5-(4-nitrophenyl)pyrimidine-2,4,6-triamine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of diaminopyrimidines as growth hormone secretagogue receptor (GHS-R) antagonists)

RN 861103-38-0 CAPLUS

CN 2,4,6-Pyrimidinetriamine, 5-(4-nitrophenyl)-N4-(phenylmethyl)- (9CI) (CA INDEX NAME)

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ANSWER 17 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2005:638854 CAPLUS
DN
     143:153392
     Preparation of aryl pyrimidines as protein kinase C inhibitors
ΤI
     Fleming, Paul E.; Shi, Zhan; Chen, Shaowu; Schmidt, Jane F.; Reader, John
IN
     C.; Hone, Neal D.; Ciavarri, Jefrey P.
     Millennium Pharmaceuticals, Inc., USA; Millennium Pharm Inc
PA
SO
     PCT Int. Appl., 177 pp.
     CODEN: PIXXD2
DT
     Patent
LА
     English
FAN.CNT 1
                               DATE
     PATENT NO.
                         KIND
                                             APPLICATION NO.
                                                                     DATE
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PΙ
     WO 2005066139
                          A2
                                 20050721
                                             WO 2005-US663
                                                                     20050110
     WO 2005066139
                          A3
                                 20051013,
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TA, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
             MR, NE, SN, TD, TĞ
     US 2006040968
                                 20060223
                                             US 2005-32299
                                                                     20050110
                          A1
PRAI US 2004-534898P
                          Ρ
                                 20040108
OS
     MARPAT 143:153392
     Title compds. I [R1 and R2 independently = H, alkyl, cycloalkyl; R3 = H or
AΒ
     F; R4 = H, F, C(0)R, etc., or R3 and R4 together = carbonyl; R = H, alkyl,
     cycloalkyl; ring A is optionally substituted with R5; R5 = halo, CN,
     aliphatic, etc.; Cyl = (un)substituted 6-membered aryl or heteroaryl,
     5-membered heteroaryl; Q = bond, CH2, CO; Cy2 = (un)substituted aryl,
     heteroaryl, heterocycle] and their pharmaceutically acceptable salts, are
     prepared and disclosed as protein kinase C (PKC) inhibitors. Thus, e.g., II
     was prepared by coupling of (3-{[3-(2-chloro-pyrimidin-4-yl)-benzyl]-ethyl-
     amino}-propyl)carbamic acid tert-Bu ester (preparation given) with tyramine and
     subsequent deprotection. The inhibitory activity of I against PKC-theta
     isoform was evaluated in an enzyme assay following the emission of
     europium cryptate (at 615 nm) and streptavidin-allophycocyanin (at 665 nm)
     and it was revealed that selected compds. of the invention display IC50
     values less than 100 nM. I as PKC inhibitor should prove useful in the
     treatment of inflammatory diseases such as, but not limited to, rheumatoid
     arthritis, asthma, and multiple sclerosis. Pharmaceutical compns.
     comprising I are disclosed.
IT
     859513-71-6P 859513-88-5P 859513-93-2P
     859513-95-4P 859514-05-9P 859514-07-1P
     859514-13-9P 859514-24-2P 859514-32-2P
     859514-46-8P 859514-64-0P 859514-76-4P
     859514-78-6P 859514-84-4P 859514-85-5P
     859515-07-4P 859515-15-4P 859515-18-7P
     859515-24-5P 859515-52-9P 859515-57-4P
     RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
```

(preparation of aryl pyrimidines as protein kinase C inhibitors)

RN 859513-71-6 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 859513-88-5 CAPLUS

CN Carbamic acid, [3-[[3-[2-[[2-(4-hydroxy-3-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl] (methylsulfonyl)amino]propyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 859513-93-2 CAPLUS

CN Carbamic acid, [3-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl](methylsulfonyl)amino]propyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 859513-95-4 CAPLUS

CN Carbamic acid, [3-[[3-[2-[[2-(3-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl] (methylsulfonyl)amino]propyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 859514-05-9 CAPLUS

CN Carbamic acid, [3-[[[3-[2-[[2-(3-bromo-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl] (methylsulfonyl)amino]propyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

O Me-S=O NH-CH₂-CH₂

$$t$$
-BuO-C-NH-(CH₂) 3-N-CH₂

RN 859514-07-1 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 859514-13-9 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[3-[2-[[2-(4-hydroxy-3-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 859514-24-2 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 859514-32-2 CAPLUS

CN Phenol, 4-[2-[[4-(3-nitrophenyl)-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859514-46-8 CAPLUS

CN Benzoic acid, 3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 859514-64-0 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-3-methyl-, 1,1-dimethylethyl ester, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859514-76-4 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-3-pyrrolidinyl- (9CI) (CA INDEX NAME)

RN 859514-78-6 CAPLUS

CN 2-Pyrimidinamine, 4-[3-[(ethylamino)methyl]phenyl]-N-[2-(3-fluorophenyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ \text{EtNH}-\text{CH}_2 & & \\ \end{array} \\ \text{EtNH}-\text{CH}_2 \\ \end{array} \\ \begin{array}{c|c} & & \\ \text{F} \\ \end{array}$$

RN 859514-84-4 CAPLUS

CN 1,3-Propanediamine, N-[1-[3-[2-[[2-(4-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

RN 859514-85-5 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[1-[3-[2-[[2-(4-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

RN 859515-07-4 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[[3-(diethylamino)propyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$_{\rm Et_2N-~(CH_2)~3-NH-CH_2}$$
 $_{\rm N}^{\rm N}$ $_{\rm NH-CH_2-CH_2}$ $_{\rm OH}$

RN 859515-15-4 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[[(1-methylethyl)amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{C1} & \text{OH} \\ \\ \text{i-PrNH-CH}_2 & \text{NH-CH}_2 - \text{CH}_2 \end{array}$$

RN 859515-18-7 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[3-[5-fluoro-2-[[2-(3-fluoro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl] (methylsulfonyl)amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

O
S
$$CH_2-CH_2-NH$$
 CH_2-NH
 C

PAGE 1-B

-- OBu-t

RN 859515-24-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-5-fluoro-4-pyrimidinyl]phenyl]methyl] (methylsul fonyl)amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

O
S
$$CH_2-CH_2-NH$$
 CH_2-CH_2-NH
 CH_2-NH
 CH_2-NH

PAGE 1-B

—oBu−t

RN 859515-52-9 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-4-piperidinyl- (9CI) (CA INDEX NAME)

RN 859515-57-4 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[(ethyl-4-piperidinylamino)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{C1} & \text{C1} \\ \text{N} & \text{NH-CH}_2 - \text{CH}_2 \end{array}$$

IT 859513-70-5P 859513-72-7P 859513-73-8P 859513-74-9P 859513-75-0P 859513-76-1P 859513-77-2P 859513-78-3P 859513-79-4P 859513-82-9P 859513-83-0P 859513-84-1P 859513-85-2P 859513-90-9P 859513-91-0P 859513-92-1P 859513-94-3P 859513-96-5P 859513-97-6P 859513-98-7P 859513-99-8P 859514-00-4P 859514-01-5P 859514-02-6P 859514-03-7P 859514-04-8P 859514-06-0P 859514-10-6P 859514-16-2P 859514-22-0P 859514-23-1P 859514-25-3P 859514-26-4P 859514-27-5P 859514-28-6P 859514-29-7P 859514-30-0P 859514-31-1P 859514-33-3P 859514-34-4P 859514-35-5P 859514-36-6P 859514-37-7P 859514-38-8P 859514-39-9P 859514-40-2P 859514-41-3P 859514-42-4P 859514-43-5P 859514-44-6P 859514-45-7P 859514-47-9P 859514-48-0P 859514-49-1P 859514-50-4P 859514-51-5P 859514-52-6P 859514-53-7P 859514-54-8P 859514-55-9P 859514-56-0P 859514-57-1P 859514-58-2P 859514-60-6P 859514-61-7P 859514-62-8P 859514-63-9P 859514-65-1P 859514-66-2P 859514-67-3P 859514-68-4P 859514-69-5P 859514-70-8P 859514-72-0P 859514-73-1P 859514-74-2P 859514-75-3P 859514-77-5P 859514-79-7P 859514-80-0P 859514-81-1P 859514-82-2P 859514-83-3P 859514-86-6P 859514-87-7P 859514-88-8P 859514-89-9P 859514-90-2P 859514-91-3P 859514-92-4P 859514-93-5P 859514-94-6P 859514-95-7P 859514-96-8P 859514-97-9P 859514-98-0P 859514-99-1P 859515-00-7P 859515-01-8P 859515-02-9P 859515-03-0P 859515-04-1P

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859515-05-2P 859515-08-5P 859515-09-6P
859515-10-9P 859515-11-0P 859515-12-1P
859515-14-3P 859515-16-5P 859515-17-6P
859515-19-8P 859515-20-1P 859515-21-2P
859515-22-3P 859515-23-4P 859515-25-6P
859515-26-7P 859515-27-8P 859515-28-9P
859515-29-0P 859515-30-3P 859515-31-4P
859515-32-5P 859515-33-6P 859515-34-7P
859515-35-8P 859515-36-9P 859515-37-0P
859515-38-1P 859515-39-2P 859515-40-5P
859515-41-6P 859515-42-7P 859515-43-8P
859515-44-9P 859515-45-0P 859515-46-1P
859515-47-2P 859515-48-3P 859515-49-4P
859515-50-7P 859515-51-8P 859515-53-0P
859515-54-1P 859515-55-2P 859515-56-3P
859515-58-5P 859515-61-0P 859515-63-2P
859515-64-3P 859515-65-4P 859515-66-5P
859515-67-6P 859515-68-7P 859515-69-8P
859515-70-1P 859515-71-2P 859515-73-4P
859515-75-6P 859515-77-8P 859515-78-9P
859515-79-0P 859515-80-3P 859515-81-4P
859515-82-5P 859515-83-6P 859515-84-7P
859515-85-8P 859515-86-9P 859515-87-0P
859515-88-1P 859515-90-5P 859515-91-6P
859515-92-7P 859515-93-8P 859515-94-9P
859515-95-0P 859515-96-1P 859515-98-3P
859515-99-4P 859516-00-0P 859516-01-1P
859516-02-2P 859516-03-3P 859516-05-5P
859516-06-6P 859516-07-7P 859516-08-8P
859516-09-9P 859516-10-2P 859516-11-3P
859516-12-4P 859516-13-5P 859516-14-6P
859516-15-7P 859516-16-8P 859516-17-9P
859516-18-0P 859516-19-1P 859516-20-4P
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859516-25-9P 859516-26-0P 859516-28-2P
859516-29-3P 859516-32-8P 859516-33-9P
859516-34-0P 859516-35-1P 859516-36-2P
859516-37-3P 859516-38-4P 859516-39-5P
859516-40-8P 859516-41-9P 859516-42-0P
859516-43-1P 859516-44-2P 859516-45-3P
859516-46-4P 859516-47-5P 859516-48-6P
859516-49-7P 859516-50-0P 859516-51-1P
859516-52-2P 859516-53-3P 859516-54-4P
859516-55-5P 859516-59-9P 859516-60-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)
    (preparation of aryl pyrimidines as protein kinase C inhibitors)
859513-70-5 CAPLUS
Phenol, 4-[2-[[4-[3-[[(3-aminopropyl)ethylamino]methyl]phenyl]-2-
pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)
```

RN

CN

RN 859513-72-7 CAPLUS

CN Acetamide, N-[4-[2-[[4-[3-[[(3-aminopropyl) (methylsulfonyl)amino]methyl]ph enyl]-2-pyrimidinyl]amino]ethyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859513-73-8 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-[4-[(methylsulfonyl)amino]phenyl]ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-(9CI) (CA INDEX NAME)

Me-
$$s$$
—NH

CH2

CH2

NH

O

S-Me

CH2-N-(CH2)3-NH2

RN 859513-74-9 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(4-aminophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-(3-aminopropyl)- (9CI) (CA INDEX NAME)

RN 859513-75-0 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(3,4-dihydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

Me-s=0 N NH-CH₂-CH₂OH

$$H_2N-(CH_2)_3-N-CH_2$$

RN 859513-76-1 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(3,4-dihydroxyphenyl)ethyl]methylamino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 859513-77-2 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(3-hydroxy-4-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me-S} \\ \text{Me-S} \\ \text{N} \\ \text{NH-CH}_2 \\ \text{CH}_2 \\ \text{NH-CH}_2 \\ \text{CH}_2 \\ \text{NH-CH}_2 \\ \text{N$$

RN 859513-78-3 CAPLUS

CN

Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[(4-hydroxyphenyl)methyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 859513-79-4 CAPLUS

CN Benzenesulfonamide, 4-[2-[[4-[3-[[(3-aminopropyl) (methylsulfonyl)amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$O = S - NH_{2}$$

$$CH_{2}$$

$$CH_{2}$$

$$CH_{2}$$

$$NH$$

$$O = S - Me$$

$$CH_{2} - N - (CH_{2})_{3} - NH_{2}$$

RN 859513-82-9 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(4-hydroxy-3,5-dimethoxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{OMe} \\ & \text{N} \\ & \text{NH-CH}_2\text{-}\text{CH}_2 \\ & \text{OMe} \\ \end{array}$$

RN 859513-83-0 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[(2-phenylethyl)amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$Me - S = O$$

$$H_2N - (CH_2)_3 - N - CH_2$$

$$N$$

$$NH - CH_2 - CH_2 - Ph$$

RN 859513-84-1 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(4-fluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 859513-85-2 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[(4-hydroxy-3-methoxyphenyl)methyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ Me-S=O \\ H_2N-(CH_2)_3-N-CH_2 \end{array} \qquad \begin{array}{c} OMe \\ N \\ NH-CH_2 \end{array}$$

RN 859513-90-9 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(4-hydroxy-3-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{OMe} \\ \text{Me-S=O} \\ \text{H}_2\text{N-} \text{(CH}_2)} \\ \text{3-N-CH}_2 \end{array} \\ \begin{array}{c} \text{OMe} \\ \text{N} \\ \text{NH-CH}_2 \\ \text{CH}_2 \end{array}$$

RN 859513-91-0 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(4-methylphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 859513-92-1 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(4-hydroxy-3-nitrophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NO2} \\ \text{Me-S=O} \\ \text{H}_2\text{N-} \text{(CH}_2\text{)}_3 - \text{N-CH}_2 \end{array} \\ \text{NH-CH}_2 - \text{CH}_2 \\ \end{array}$$

RN 859513-94-3 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ \text{Me}-\text{S} & \text{O} & & \\ \text{H}_2\text{N}-\text{(CH}_2)} & 3-\text{N}-\text{CH}_2 & & \\ \end{array}$$

RN 859513-96-5 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(3-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 859513-97-6 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(2-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 859513-98-7 CAPLUS

CN Carbamic acid, [3-[(methylsulfonyl)[[3-[2-[[2-(3,4,5-trihydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]amino]propyl]-,

1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 859513-99-8 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(3,5-dichloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \text{C1} \\ & & & \\ \text{Me-S} & \text{O} & & \\ & & & \\ \text{H}_2\text{N}-\text{(CH}_2)_3-\text{N}-\text{CH}_2 & & \\ & & & \\ \end{array}$$

RN 859514-00-4 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(3-chlorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 859514-01-5 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(2-chlorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 859514-02-6 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(4-chlorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 859514-03-7 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(3-hydroxy-4-nitrophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ Me-S=O \\ H_2N-(CH_2)_3-N-CH_2 \end{array} \qquad \begin{array}{c} OH \\ NO_2 \\ N \end{array}$$

RN 859514-04-8 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(2,3-dihydro-2-oxo-5-benzoxazolyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ \text{Me} - & & & \\ \hline & & \\ \text{H}_2\text{N} - (\text{CH}_2)_3 - \text{N} - \text{CH}_2 \end{array} \begin{array}{c} & & \\ & & \\ \text{N} \end{array} \begin{array}{c} & \\ & & \\ \text{N} \end{array} \begin{array}{c} & \\ & \\ \text{N} \end{array} \begin{array}{c} & \\ & \\ \text{N} \end{array} \begin{array}{c} & \\ & \\ \text{O} \end{array}$$

RN 859514-06-0 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(3-bromo-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Me}-\text{S} & & & \\ & & & \\ \text{H}_2\text{N}-\text{(CH}_2)} & 3-\text{N}-\text{CH}_2 & & \\ \end{array}$$

RN 859514-10-6 CAPLUS

CN Phenol, 4-[2-[[4-[3-(4-piperidinylamino)phenyl]-2-pyrimidinyl]amino]ethyl](9CI) (CA INDEX NAME)

RN 859514-16-2 CAPLUS

CN Phenol, 2-methoxy-4-[2-[[4-[3-(4-piperidinylamino)phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OMe} \\ \text{NH} \\ \hline \\ \text{NH} \\ \hline \end{array} \begin{array}{c} \text{NH} \\ \text{NH} \\ \hline \end{array} \begin{array}{c} \text{OMe} \\ \text{CH}_2 \\ \text{CH}_2 \\ \hline \end{array}$$

RN 859514-22-0 CAPLUS

CN 2-Pyrimidinamine, N-(1-naphthalenylmethyl)-4-[3-(4-piperidinylamino)phenyl]- (9CI) (CA INDEX NAME)

RN 859514-23-1 CAPLUS

CN Phenol, 2-methoxy-5-[2-[[4-[3-(4-piperidinylamino)phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OH} & \text{OMe} \\ \hline \\ \text{NH} & \text{NH} - \text{CH}_2 - \text{CH}_2 \\ \hline \end{array}$$

RN 859514-25-3 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-(4-piperidinylamino)phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

HN NH
$$\sim$$
 NH \sim CH₂ \sim CH₂ \sim OH

RN 859514-26-4 CAPLUS

CN 2-Pyrimidinamine, N-[2-(1,3-benzodioxol-5-yl)ethyl]-4-[3-(4-piperidinylamino)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 859514-27-5 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3-fluorophenyl)ethyl]-4-[3-(4-

piperidinylamino)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} HN & NH-CH_2-CH_2 \\ \hline \end{array}$$

RN 859514-28-6 CAPLUS

CN Phenol, 2,6-dichloro-4-[2-[[4-[3-(4-piperidinylamino)phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

HN NH
$$\sim$$
 NH \sim CH₂ \sim CH₂ \sim C1 \sim

RN 859514-29-7 CAPLUS

CN Phenol, 3-[2-[[4-[3-(4-piperidinylamino)phenyl]-2-pyrimidinyl]amino]ethyl](9CI) (CA INDEX NAME)

$$^{\rm HN}$$
 $^{\rm NH}$ $^{\rm NH}$ $^{\rm CH_2}$ $^{\rm CH_2}$ $^{\rm OH}$

RN 859514-30-0 CAPLUS

CN Phenol, 2-bromo-4-[2-[[4-[3-(4-piperidinylamino)phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859514-31-1 CAPLUS

CN 2-Pyrimidinamine, N-[(6-fluoro-4H-1,3-benzodioxin-8-yl)methyl]-4-[3-(4-piperidinylamino)phenyl]- (9CI) (CA INDEX NAME)

RN 859514-33-3 CAPLUS

CN Phenol, 4-[2-[[4-[3-(3-piperidinylamino)phenyl]-2-pyrimidinyl]amino]ethyl]-(9CI) (CA INDEX NAME)

RN 859514-34-4 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-(3-piperidinylamino)phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859514-35-5 CAPLUS

CN Phenol, 4-[2-[[4-[3-(3-pyrrolidinylamino)phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859514-36-6 CAPLUS

CN Benzamide, N-[3-[[[3-[2-([2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl](methylsulfonyl)amino]propyl]- (9CI) (CA INDEX NAME)

RN 859514-37-7 CAPLUS

CN Benzamide, N-[3-[[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl](methylsulfonyl)amino]propyl]-2-methyl- (9CI) (CA INDEX NAME)

PAGE 1-B

__ OH

RN 859514-38-8 CAPLUS

CN Benzamide, 4-chloro-N-[3-[[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl](methylsulfonyl)amino]propyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

RN 859514-39-9 CAPLUS

CN Benzamide, N-[3-[[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl](methylsulfonyl)amino]propyl]-4-methyl- (9CI) (CA INDEX NAME)

PAGE 1-B

RN 859514-40-2 CAPLUS

CN 2-Pyridinecarboxamide, N-[3-[[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl] (methylsulfonyl)amino]propyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

__ OH

RN 859514-41-3 CAPLUS

CN Benzamide, 3-chloro-N-[3-[[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl] (methylsulfonyl)amino]propyl]- (9CI) (CA INDEX NAME)

C1
$$0 \text{ Me} - \text{S} = 0$$
 $0 \text{ NH} - \text{CH}_2 - \text{CH}_2$ $0 \text{ NH} - \text{CH}_2 - \text{CH}_2$

PAGE 1-B

RN 859514-42-4 CAPLUS

CN 3-Pyridinecarboxamide, N-[3-[[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl](methylsulfonyl)amino]propyl]-2-methyl- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

__ OH

RN 859514-43-5 CAPLUS

CN Benzamide, N-[3-[[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl](methylsulfonyl)amino]propyl]-2-methoxy- (9CI) (CA INDEX NAME)

PAGE 1-B

__ OH

RN 859514-44-6 CAPLUS

CN Benzenemethanesulfonamide, N-[3-[[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl](methylsulfonyl)amino]propyl]- (9CI) (CA INDEX NAME)

RN 859514-45-7 CAPLUS

CN Benzenesulfonamide, N-[3-[[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl](methylsulfonyl)amino]propyl]- (9CI) (CA INDEX NAMÉ)

RN 859514-47-9 CAPLUS

CN Benzamide, 3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]-N-(3-pyrrolidinylmethyl)- (9CI) (CA INDEX NAME)

RN 859514-48-0 CAPLUS

CN Benzamide, N-(3-aminopropyl)-3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 859514-49-1 CAPLUS

CN Benzamide, 3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]-N-(2-piperidinylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & &$$

RN 859514-50-4 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-(2-pyridinylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & O \\
 & N \\
 & N \\
 & CH_2 - N - CH_2
\end{array}$$

$$\begin{array}{c|c}
 & O \\
 & N \\
 & NH - CH_2 - CH_2
\end{array}$$

$$\begin{array}{c|c}
 & OH \\
 & NH - CH_2 - CH_2
\end{array}$$

RN 859514-51-5 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-(3-pyridinylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & O \\
 & Me-s = O \\
 & N \\
 & CH_2-N-CH_2 \\
 & N \\
 & NH-CH_2-CH_2
\end{array}$$
OH

RN 859514-52-6 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-(4-pyridinylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & O \\
 & Me-S=O \\
 & CH_2-N-CH_2 \\
 & NH-CH_2-CH_2
\end{array}$$
OH

RN 859514-53-7 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-[2-(2-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O \\ \hline N \\ \hline Me-S \\ \hline O \\ CH_2-CH_2-N-CH_2 \\ \hline \end{array} \begin{array}{c} N \\ \hline N \\ NH-CH_2-CH_2 \\ \hline \end{array} \begin{array}{c} OH \\ \hline \end{array}$$

RN 859514-54-8 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-[2-(3-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ N & & & \\ \hline \\ N & & \\ \end{array} \begin{array}{c} \text{CH}_2 - \text{CH}_2 - \text{CH}_2 \\ \hline \\ \end{array} \begin{array}{c} \text{OH} \\ \\ N & \\ \end{array} \begin{array}{c} \text{OH} \\ \\ N & \\ \end{array}$$

RN 859514-55-9 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-[2-(4-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & O \\
 & Me-s = O \\
 & CH_2-CH_2-N-CH_2
\end{array}$$

$$\begin{array}{c|c}
 & N \\
 & NH-CH_2-CH_2
\end{array}$$

RN 859514-56-0 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[ethyl(3-pyridinylmethyl)amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859514-57-1 CAPLUS

CN Propanamide, 3-amino-N-[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859514-58-2 CAPLUS

CN 3-Pyridinepropanamide, N-[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859514-60-6 CAPLUS

CN Benzenemethanesulfonamide, N-[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859514-61-7 CAPLUS

CN Phenol, 4-[2-[[4-[3-[ethyl(3-pyridinylmethyl)amino]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859514-62-8 CAPLUS

CN Phenol, 4-[2-[[4-[3-[(4-methyl-1-piperazinyl)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Me N NH
$$CH_2$$
 N NH CH_2 CH_2

RN 859514-63-9 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-3-methyl-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859514-65-1 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859514-66-2 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(2R)-2-methyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859514-67-3 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-4-piperidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ HN & & S = O & \\ N-CH_2 & & NH-CH_2-CH_2 \end{array}$$
 OH

RN 859514-68-4 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(3-fluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-4-piperidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ HN & & S = O \\ \hline N & & NH-CH_2-CH_2 \end{array}$$

RN 859514-69-5 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[(2-phenylethyl)amino]-4-pyrimidinyl]phenyl]methyl]-N-4-piperidinyl- (9CI) (CA INDEX NAME)

RN 859514-70-8 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(3-chlorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-4-piperidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & O \\
 & \parallel \\
 & N \\$$

RN 859514-72-0 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(4-hydroxy-3-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-4-piperidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O \\ \hline \\ HN & Me-S = O \\ \hline \\ N-CH_2 & NH-CH_2-CH_2 \end{array} \begin{array}{c} OMe \\ OH \\ \hline \end{array}$$

RN 859514-73-1 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-3-piperidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ \hline Me-s=0 & \\ \hline N & NH-CH_2-CH_2 \end{array}$$

RN 859514-74-2 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(4-hydroxy-3-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-3-piperidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O \\ \hline Me-S & O \\ \hline N & NH-CH_2-CH_2 \\ \hline \end{array}$$

RN 859514-75-3 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-(4-piperidinylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ Me-s=0 & & & \\ CH_2-N-CH_2 & & & N \\ \end{array}$$

RN 859514-77-5 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[(ethylamino)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{C1} & \text{OH} \\ \hline \\ \text{EtNH-CH}_2 & \text{CH}_2 & \text{CH}_2 \\ \hline \end{array}$$

RN 859514-79-7 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-ethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ Me-S=O \\ Et-N-CH_2 \end{array} \begin{array}{c} OH \\ N \\ NH-CH_2-CH_2 \end{array}$$

RN 859514-80-0 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[[ethyl(1-methylethyl)amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{C1} \\ \text{i-Pr-N-CH}_2 & \text{N} \\ \end{array}$$

RN 859514-81-1 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[[ethyl(3-methylbutyl)amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{C1} \\ & \text{N} \\ \text{Me2CH-CH2-CH2-N-CH2} \end{array} \\ \begin{array}{c|c} \text{OH} \\ & \text{N} \end{array}$$

RN 859514-82-2 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[[ethyl(2-methylpropyl)amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{N} \\ \text{i-Bu-N-CH}_2 \end{array} \text{OH}$$

RN 859514-83-3 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[(ethylpropylamino)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{N} \\ \text{NH-CH}_2\text{-CH}_2 \end{array}$$

RN 859514-86-6 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[1-[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]ethyl]- (9CI) (CA INDEX NAME)

RN 859514-87-7 CAPLUS

CN Benzamide, N-[3-[ethyl[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]amino]propyl]- (9CI) (CA INDEX NAME)

RN 859514-88-8 CAPLUS

CN Phenol, 4-[2-[[4-[3-(1-methylethoxy)phenyl]-2-pyrimidinyl]amino]ethyl]-(9CI) (CA INDEX NAME)

RN 859514-89-9 CAPLUS

CN Phenol, 2-methoxy-4-[2-[[4-[3-(1-methylethoxy)phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OPr-i} & \text{OMe} \\ \hline \\ N & \text{NH-} \text{CH}_2\text{--} \text{CH}_2 \\ \hline \end{array}$$

RN 859514-90-2 CAPLUS

CN Phenol, 4-[2-[[4-(3-butoxyphenyl)-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859514-91-3 CAPLUS

CN Phenol, 4-[2-[[4-(3-butoxyphenyl)-2-pyrimidinyl]amino]ethyl]-2-methoxy-(9CI) (CA INDEX NAME)

$$\begin{picture}(20,0) \put(0,0){\line(0,0){100}} \put(0,0){\line(0,0){100$$

RN 859514-92-4 CAPLUS

CN Phenol, 4-[2-[[4-(4-ethoxyphenyl)-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859514-93-5 CAPLUS

CN Phenol, 4-[2-[[4-(4-ethoxyphenyl)-2-pyrimidinyl]amino]ethyl]-2-methoxy-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{OMe} & \text{OMe} \\ \hline \\ N & \text{NH-} \text{CH}_2\text{-} \text{CH}_2 \\ \hline \end{array}$$

RN 859514-94-6 CAPLUS

CN Carbamic acid, [4-[2-[[2-(4-hydroxy-3-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 859514-95-7 CAPLUS

CN Phenol, 2-methoxy-4-[2-[[4-[4-(2-methylpropyl)phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\text{i-Bu} \qquad \qquad \text{OMe} \qquad \text{OH} \qquad \qquad \text{O$$

RN 859514-96-8 CAPLUS

CN Phenol, 2-methoxy-4-[2-[[4-(4-propoxyphenyl)-2-pyrimidinyl]amino]ethyl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{OMe} \\ \text{N} \\ \text{NH-CH}_2\text{-CH}_2 \end{array} \begin{array}{c} \text{OMe} \\ \text{OH} \\ \text{OH$$

RN 859514-97-9 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-3-piperidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

RN 859514-98-0 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-3-pyrrolidinyl- (9CI) (CA INDEX NAME)

RN 859514-99-1 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-(4-piperidinylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ Me-S = O \\ CH_2-N-CH_2 \\ \end{array} \begin{array}{c} OH \\ NH-CH_2-CH_2 \\ \end{array}$$

RN 859515-00-7 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-[2-(2-piperidinyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & C1 \\ NH & Me-S=O \\ CH_2-CH_2-N-CH_2 \\ \hline \end{array} \begin{array}{c} NH - CH_2-CH_2 \\ \hline \end{array} \begin{array}{c} OH \\ NH-CH_2-CH_2 \\ \hline \end{array}$$

RN 859515-01-8 CAPLUS

CN 1,3-Propanediamine, N-ethyl-N-[[3-[2-[[2-(4-methoxy-3-methylphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ & \text{N} \\ \text{H}_2\text{N}-\text{(CH}_2)} & \text{3}-\text{N}-\text{CH}_2 \end{array} \\ \begin{array}{c|c} \text{OMe} \\ & \text{N} \end{array}$$

RN 859515-02-9 CAPLUS

CN Acetamide, N-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-(3-pyrrolidinylmethyl)- (9CI) (CA INDEX NAME)

RN 859515-03-0 CAPLUS

CN Benzenemethanol, $3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]-\alpha-methyl- (9CI) (CA INDEX NAME)$

RN 859515-04-1 CAPLUS

CN Phenol, 4-[2-[[4-[3-[(pyrazinylamino)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859515-05-2 CAPLUS

CN Phenol, 4-[2-[[4-[3-[(3-pyridinylamino)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$N$$
 $NH-CH_2$
 $NH-CH_2-CH_2$
 $NH-CH_2-CH_2$

RN 859515-08-5 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[[3-(diethylamino)propyl]ethylamino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859515-09-6 CAPLUS

CN Phenol, 4-[2-[[4-[4-[[(1-methylethyl)amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859515-10-9 CAPLUS

CN 3-Piperidinecarboxamide, N-ethyl-N-[[3-[2-[[2-(3-fluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859515-11-0 CAPLUS

CN 3-Piperidinecarboxamide, N-ethyl-N-[[3-[2-[[2-(3-fluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859515-12-1 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3-fluorophenyl)ethyl]-4-[3-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859515-14-3 CAPLUS

CN Phenol, 4-[2-[[4-[3-[(ethylamino)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859515-16-5 CAPLUS

CN Piperazinone, 1-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-4,6-dimethyl-, (6S)- (9CI) (CA INDEX NAME)

RN 859515-17-6 CAPLUS

CN Methanesulfonamide, N-[[3-[5-fluoro-2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-4-piperidinyl- (9CI) (CA INDEX NAME)

HO
$$O = S - Me$$
 NH $CH_2 - CH_2 - NH$ NH

RN 859515-19-8 CAPLUS

CN Methanesulfonamide, N-[[3-[5-fluoro-2-[[2-(3-fluoro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-4-piperidinyl-(9CI) (CA INDEX NAME)

HO
$$CH_2-CH_2-NH$$

$$N$$

$$CH_2-NH$$

$$NH$$

$$CH_2-NH$$

$$NH$$

RN 859515-20-1 CAPLUS

CN Methanesulfonamide, N-[[3-[5-fluoro-2-[[2-(3-fluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-4-piperidinyl- (9CI) (CA INDEX NAME)

$$CH_2-CH_2-NH$$

$$CH_2-CH_2-NH$$

$$CH_2-NH$$

$$CH_2-NH$$

$$CH_2-NH$$

$$CH_2-NH$$

RN 859515-21-2 CAPLUS

CN Methanesulfonamide, N-[[3-[5-fluoro-2-[[2-(4-hydroxy-3-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-4-piperidinyl-(9CI) (CA INDEX NAME)

HO OME
$$CH_2-CH_2-NH$$
 NH CH_2-NH NH

RN 859515-22-3 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(3-chlorophenyl)ethyl]amino]-5-fluoro-4-pyrimidinyl]phenyl]methyl]-N-4-piperidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ \hline & & & \\ \hline & & \\ C1 & & \\ \hline \end{array} \qquad \begin{array}{c} CH_2-CH_2-NH & \\ \hline & \\ N & \\ \hline \end{array} \qquad \begin{array}{c} CH_2-NH & \\ \hline \end{array} \qquad \begin{array}{c} NH & \\ \hline \\ CH_2-NH & \\ \hline \end{array} \qquad \begin{array}{c} NH & \\ \hline \\ NH & \\ \hline \end{array}$$

RN 859515-23-4 CAPLUS

CN Methanesulfonamide, N-[[3-[5-fluoro-2-[(2-phenylethyl)amino]-4-pyrimidinyl]phenyl]methyl]-N-4-piperidinyl- (9CI) (CA INDEX NAME)

RN 859515-25-6 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-5-fluoro-4-pyrimidinyl]phenyl]methyl]-N-4-piperidinyl- (9CI) (CA INDEX NAME)

HO CH₂-CH₂-NH NH
$$CH_2$$
-NH CH_2 -NH CH_2 -NH

RN 859515-26-7 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(3-aminopropyl)ethylamino]methyl]phenyl]-5-fluoro-2-pyrimidinyl]amino]ethyl]-2-fluoro- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Et} & & & \\ \text{H}_2\text{N}-\text{(CH}_2)} & 3-\text{N}-\text{CH}_2 & & \\ \end{array}$$

RN 859515-27-8 CAPLUS

CN 1,3-Propanediamine, N-ethyl-N-[[3-[5-fluoro-2-[[2-(3-fluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 859515-28-9 CAPLUS

CN 1,3-Propanediamine, N-[[3-[2-[[2-(3-chlorophenyl)ethyl]amino]-5-fluoro-4-pyrimidinyl]phenyl]methyl]-N-ethyl- (9CI) (CA INDEX NAME)

RN 859515-29-0 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(3-aminopropyl)ethylamino]methyl]phenyl]-5-fluoro-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859515-30-3 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(3-aminopropyl)ethylamino]methyl]phenyl]-5-fluoro-2-pyrimidinyl]amino]ethyl]-2-chloro- (9CI) (CA INDEX NAME)

RN 859515-31-4 CAPLUS

CN Phenol, 4-[2-[[5-fluoro-4-[3-[2-(4-piperidinyl)ethyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\mathsf{CH}_2 - \mathsf{CH}_2 - \mathsf{NH} - \mathsf{NH} - \mathsf{CH}_2 - \mathsf{CH}_2 - \mathsf{CH}_2$$

RN 859515-32-5 CAPLUS

CN Phenol, 2-chloro-4-[2-[[5-fluoro-4-[3-[2-(4-piperidinyl)ethyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

HO
$$CH_2-CH_2-NH$$
 NH CH_2-CH_2 NH

RN 859515-33-6 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-(4-piperidinylamino)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ &$$

RN 859515-34-7 CAPLUS

CN Phenol, 2-fluoro-4-[2-[[4-[3-(4-piperidinylamino)phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

HN NH
$$\sim$$
 NH \sim CH₂ \sim CH₂ \sim OH

RN 859515-35-8 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[(ethyl-4-piperidinylamino)methyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ \text{HN} & & \\ &$$

RN 859515-36-9 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859515-37-0 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859515-38-1 CAPLUS

CN 2-Pyrimidinamine, 4-[3-[(ethyl-4-piperidinylamino)methyl]phenyl]-N-[2-(3-fluorophenyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{HN} & \text{Et} \\ \hline & \text{N} - \text{CH}_2 \\ \hline & \text{N} \\ \end{array}$$

RN 859515-39-2 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-(1-ethyl-4-piperidinyl)- (9CI) (CA INDEX NAME)

Et
$$N = S = O$$
 $N = CH_2 = CH_2 = OH$

RN 859515-40-5 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-(1-propyl-4-piperidinyl)- (9CI) (CA INDEX NAME)

RN 859515-41-6 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[[ethyl(1-ethyl-4-piperidinyl)amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859515-42-7 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[[ethyl(1-propyl-4-piperidinyl)amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{C1} & \text{OH} \\ & \text{N} & \text{NH- CH}_2-\text{CH}_2 \end{array}$$

RN 859515-43-8 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[[ethyl[1-(4-pyridinylmethyl)-4-piperidinyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-B

__ OH

RN 859515-44-9 CAPLUS

CN Methanesulfonamide, N-[[5-[2-[[2-(3-fluorophenyl)ethyl]amino]-4-pyrimidinyl]-2-methoxyphenyl]methyl]-N-4-piperidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ \hline \\ HN & \\ \hline \\ Me - S = O \\ \hline \\ N - CH_2 & \\ \hline \\ MeO & \\ \end{array}$$

RN 859515-45-0 CAPLUS

CN Methanesulfonamide, N-[[2-methoxy-5-[2-[(2-phenylethyl)amino]-4-pyrimidinyl]phenyl]methyl]-N-4-piperidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & O \\ \hline O & S-Me \\ \hline OH_2-CH_2-NH & NH \\ \hline OMe \\ \end{array}$$

RN 859515-46-1 CAPLUS

CN Methanesulfonamide, N-[[5-[2-[[2-(3-fluoro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]-2-methoxyphenyl]methyl]-N-4-piperidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ HN & Me-S = O & & N \\ N-CH_2 & & NH-CH_2-CH_2 \end{array}$$
 OH

RN 859515-47-2 CAPLUS

CN Methanesulfonamide, N-[[2-fluoro-5-[2-[[2-(3-fluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-4-piperidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ \parallel & \\ N-CH_2 & \\ \end{array}$$

$$N - CH_2 - CH_2$$

RN 859515-48-3 CAPLUS

CN Methanesulfonamide, N-[[2-fluoro-5-[2-[[2-(3-fluoro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-4-piperidinyl-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ &$$

RN 859515-49-4 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[ethyl(1-propyl-4-piperidinyl)amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]-2-fluoro- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} n-\text{Pr} & & \text{F} \\ & N & \text{NH}-\text{CH}_2-\text{CH}_2 \\ \hline \end{array}$$

RN 859515-50-7 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[ethyl[1-(4-pyridinylmethyl)-4-piperidinyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]-2-fluoro-(9CI) (CA INDEX NAME)

PAGE 1-B

__ OH

RN 859515-51-8 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(3-fluoro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-4-piperidinyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & & \\ HN & Me-S & O & & & \\ N-CH_2 & & & NH-CH_2-CH_2 & & \\ \end{array}$$

RN 859515-53-0 CAPLUS

CN Phenol, 2-fluoro-4-[2-[[4-[3-[(4-piperidinylpropylamino)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ \text{HN} & & \text{Pr-n} & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\$$

RN 859515-54-1 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[(4-piperidinylpropylamino)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ \text{HN} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 859515-55-2 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3-fluorophenyl)ethyl]-4-[3-[(4-piperidinylpropylamino)methyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \operatorname{HN} & \operatorname{Pr-n} & \\ & \operatorname{N-CH_2} & \\ & \operatorname{NH-CH_2-CH_2} \end{array}$$

RN 859515-56-3 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[2-(4-piperidinyl)ethyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

HO
$$CH_2-CH_2-NH$$
 NH CH_2-CH_2 NH

RN 859515-58-5 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[ethyl](3S)-3-piperidinylmethyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859515-61-0 CAPLUS

CN Phenol, 4-[2-[[4-[3-[(ethyl-4-piperidinylamino)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{HN} & \text{Et} \\ \hline & \text{N} \\ \hline & \text{N} \\ \end{array} \begin{array}{c} \text{OH} \\ \hline \end{array}$$

RN 859515-63-2 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[[2-(1-methylethyl)-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859515-64-3 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-5-fluoro-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me-S} \\ \text{O} \\ \text{H}_2\text{N}-\text{(CH}_2)} \\ \text{3}-\text{N}-\text{CH}_2 \end{array} \begin{array}{c} \text{F} \\ \text{N} \\ \text{N} \end{array} \text{NH-CH}_2-\text{CH}_2 \end{array}$$

RN 859515-65-4 CAPLUS

CN Phenol, 2-methyl-4-[2-[[4-[3-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859515-66-5 CAPLUS

CN Phenol, 4-[2-[[4-[3-[(3-azetidinylethylamino)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859515-67-6 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[2-(1-methylethyl)-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{i-Pr} \\ \text{N} \\ \text{CH}_2 \\ \end{array} \begin{array}{c} \text{N} \\ \text{N} \\ \end{array} \begin{array}{c} \text{NH-CH}_2 \\ \text{CH}_2 \\ \end{array} \begin{array}{c} \text{OH} \\ \end{array}$$

RN 859515-68-7 CAPLUS

CN 1-Naphthalenol, 4-[2-[[4-[3-[(ethyl-4-piperidinylamino)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859515-69-8 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[ethyl[2-(2S)-2-pyrrolidinylethyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859515-70-1 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[[(2S)-2-methyl-1-piperidinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859515-71-2 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(3S)-3-(1H-indol-3-ylmethyl)-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859515-73-4 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(3R)-3-(phenylmethyl)-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859515-75-6 CAPLUS

CN Phenol, 3-[2-[[4-[3-[[ethyl[2-(2S)-2-pyrrolidinylethyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859515-77-8 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[(2R)-2-methyl-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859515-78-9 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[5-fluoro-2-[[2-(3-fluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 859515-79-0 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[(2S)-2-ethyl-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859515-80-3 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[(2R)-2-ethyl-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859515-81-4 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(3S)-3-(2-methylpropyl)-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859515-82-5 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3-fluorophenyl)ethyl]-4-[3-[2-(4-piperidinyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \mathsf{HN} & \mathsf{N} \\ \mathsf{CH_2} - \mathsf{CH_2} \\ \hline \end{array} \qquad \begin{array}{c|c} \mathsf{N} \\ \mathsf{NH} - \mathsf{CH_2} - \mathsf{CH_2} \\ \hline \end{array}$$

RN 859515-83-6 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[(2R,6S)-2,6-dimethyl-1-piperazinyl]methyl]phenyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859515-84-7 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[2-[[2-(3-chlorophenyl)ethyl]amino]-5-fluoro-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 859515-85-8 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl-2,2-d2]-4-[3-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859515-86-9 CAPLUS

CN 2-Pyrimidinamine, 4-[3-[(3-azetidinylethylamino)methyl]phenyl]-N-[2-(3,5-difluorophenyl)ethyl-2,2-d2]- (9CI) (CA INDEX NAME)

RN 859515-87-0 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[2-(1-methylethyl)-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859515-88-1 CAPLUS

CN 2-Pyrimidinamine, 4-[3-[(ethyl-4-piperidinylamino)methyl]phenyl]-N-[2-[3-(trifluoromethyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \operatorname{HN} & \operatorname{Et} & \\ & \operatorname{N-CH_2} & \\ & \operatorname{NH-CH_2-CH_2} \end{array}$$

RN 859515-90-5 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3-chlorophenyl)ethyl]-5-fluoro-4-[3-[2-(4-piperidinyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

$$\mathsf{CH}_2-\mathsf{CH}_2-\mathsf{NH} - \mathsf{NH} - \mathsf{CH}_2-\mathsf{CH}_2 - \mathsf{NH}$$

RN 859515-91-6 CAPLUS

CN 2-Pyrimidinamine, 5-fluoro-N-[2-(3-fluorophenyl)ethyl]-4-[3-[2-(4-piperidinyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

$$\mathsf{CH}_2 - \mathsf{CH}_2 - \mathsf{NH} - \mathsf{NH} - \mathsf{CH}_2 - \mathsf{CH}_2 - \mathsf{CH}_2$$

RN 859515-92-7 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[(3S)-3-(1H-indol-3-ylmethyl)-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859515-93-8 CAPLUS

CN 2-Pyrimidinamine, 5-fluoro-N-(2-phenylethyl)-4-[3-[2-(4-piperidinyl)ethyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph-CH}_2\text{-CH}_2\text{-NH} \\ & \text{HN} \\ & \text{CH}_2\text{-CH}_2 \\ & \text{F} \end{array}$$

RN 859515-94-9 CAPLUS

CN 2-Pyrimidinamine, 4-[3-[(3-azetidinylethylamino)methyl]phenyl]-N-[2-(3-fluorophenyl)ethyl]- (9CI) (CA INDEX NAME)

RN 859515-95-0 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3-fluorophenyl)ethyl]-4-[3-[[2-(1-methylethyl)-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859515-96-1 CAPLUS

CN 2-Pyrimidinamine, 4-[3-[[ethyl[(3S)-3-piperidinylmethyl]amino]methyl]pheny 1]-N-[2-(3-fluorophenyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859515-98-3 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[(2-ethyl-4-methyl-1-piperazinyl)methyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & \\ & & \\ N & \\ N$$

RN 859515-99-4 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(3R)-3-phenyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859516-00-0 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[(2S)-4-ethyl-2-methyl-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859516-01-1 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(1,1-dimethylethyl)amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & \text{OH} \\ & & \text{N} \\ \text{t-BuNH-CH}_2 & \text{CH}_2 \\ \end{array}$$

RN 859516-02-2 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[[(1,1-dimethylethyl)amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$t-BuNH-CH_2$$
 N
 $NH-CH_2-CH_2$
 OH

RN 859516-03-3 CAPLUS

CN Phenol, 2-chloro-4-[[[4-[3-[[(1-methylethyl)amino]methyl]phenyl]-2-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{C1} & \text{OH} \\ \hline \text{i-PrNH-CH}_2 & \text{N} & \text{NH-CH}_2 \\ \end{array}$$

RN 859516-05-5 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3-chloro-4-methoxyphenyl)ethyl]-4-[3-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859516-06-6 CAPLUS

CN 2-Pyrimidinamine, N-[2-(4-amino-3-chlorophenyl)ethyl]-4-[3-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859516-07-7 CAPLUS

CN 3-Pyridinecarboxamide, N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-2-methyl-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 859516-08-8 CAPLUS

CN 2-Pyridinecarboxamide, N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-3-methyl-N-(1-methylethyl)-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{O} & \text{Pr-i} \\ \hline & \text{C} & \text{N} & \text{CH}_2 \\ \hline & \text{N} & \text{NH} - \text{CH}_2 - \text{CH}_2 \\ \hline \end{array}$$

RN 859516-09-9 CAPLUS

CN 3-Pyridinecarboxamide, N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-5-methyl-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 859516-10-2 CAPLUS

CN 3-Pyridinecarboxamide, N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-6-methyl-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 859516-11-3 CAPLUS

CN 4-Pyridinecarboxamide, N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-(1-methylethyl)-(9CI) (CA INDEX NAME)

RN 859516-12-4 CAPLUS

CN 3-Pyridinecarboxamide, N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-(1-methylethyl)-6-(trifluoromethyl)-(9CI) (CA INDEX NAME)

RN 859516-13-5 CAPLUS

CN 3-Pyridinecarboxamide, N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-(1-methylethyl)-4-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 859516-14-6 CAPLUS

CN 3-Pyridinecarboxamide, 5-bromo-N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-(1-methylethyl)-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \text{C1} \\ & & & \\ & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

RN 859516-15-7 CAPLUS

CN 4-Piperidinecarboxamide, N-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-1-methyl-N-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 859516-16-8 CAPLUS

CN 1H-Indole-5-ethanamine, N-[4-[3-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859516-17-9 CAPLUS

CN 1H-Indole-5-ethanamine, N-[4-[3-[(ethyl-4-piperidinylamino)methyl]phenyl]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Et} & \\ & \text{N} & \text{NH} - \text{CH}_2 - \text{CH}_2 \\ \hline & & \text{NH} \end{array}$$

RN 859516-18-0 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(3S)-3-methyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859516-19-1 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(3R)-3-methyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859516-20-4 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[(3S)-3-methyl-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859516-21-5 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[(3R)-3-methyl-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859516-22-6 CAPLUS

CN Phenol, 4-[2-[[4-[3-[(2-ethyl-1-piperazinyl)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Et} \\ \text{N} \\ \text{CH}_2 \\ \end{array} \begin{array}{c} \text{N} \\ \text{N} \\ \text{N} \\ \end{array} \begin{array}{c} \text{OH} \\ \text{CH}_2 \\ \end{array} \begin{array}{c} \text{OH} \\ \text{OH} \\ \end{array}$$

RN 859516-23-7 CAPLUS

CN Phenol, 4-[2-[[4-[3-[(2-propyl-1-piperazinyl)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{N} \\ \text{$$

RN 859516-25-9 CAPLUS

CN 2-Piperazinecarboxylic acid, 4-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{HN} & \text{N} & \text{CH}_2 & \text{OH} \\ & & & \\ & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & &$$

RN 859516-26-0 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3-chlorophenyl)ethyl]-4-[3-[(ethyl-4-piperidinylamino)methyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \operatorname{HN} & \operatorname{Et} & \operatorname{N} & \operatorname{NH-CH_2-CH_2} \\ & \operatorname{N-CH_2} & & \operatorname{C1} \end{array}$$

RN 859516-28-2 CAPLUS

CN 2-Pyrimidinamine, N-[2-(2,5-difluorophenyl)ethyl]-4-[3-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859516-29-3 CAPLUS

CN 2-Pyrimidinamine, 4-[3-[(2-ethyl-1-piperazinyl)methyl]phenyl]-N-[2-(3-fluorophenyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{HN} & \text{N} \\ \hline & \text{CH}_2 \\ \hline & \text{Et} \\ \end{array}$$

RN 859516-32-8 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[[(3S,4R)-3-methyl-4-piperidinyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859516-33-9 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[(3S,4R)-3-methyl-4-(3-[(3S,4R)-3-methyl-4-(3-(3S,4R)-3-methyl-4-(3S,4R)-3-(3S,

4-piperidinyl]amino]methyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859516-34-0 CAPLUS

CN 2-Pyrimidinamine, N-[2-(4-bromophenyl)ethyl]-4-[3-[[[(3S,4R)-3-methyl-4-piperidinyl]amino]methyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859516-35-1 CAPLUS

CN 2-Piperazinecarboxylic acid, 1-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{CO}_2\text{H} \\ & \text{N} & \text{CH}_2 \\ & \text{N} & \text{NH} - \text{CH}_2 - \text{CH}_2 \\ \end{array}$$

RN 859516-36-2 CAPLUS

CN 2-Piperazinecarboxylic acid, 1-[[3-[2-[[2-(3,5-difluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$N$$
 CH_2 N NH CH_2 CH_2 F

RN 859516-37-3 CAPLUS

CN 2-Piperazinecarboxamide, 1-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 859516-38-4 CAPLUS

CN 2-Piperazinecarboxamide, 1-[[3-[2-[[2-(3-fluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ &$$

RN 859516-39-5 CAPLUS

CN 2-Piperazinecarboxamide, 1-[[3-[2-[[2-(3,5-difluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{HN} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 859516-40-8 CAPLUS

CN 2-Piperazinecarbonitrile, 4-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{NC} & \text{NH-} \text{CH}_2 - \text{CH}_2 \\ \hline & \text{NH-} \text{CH}_2 - \text{CH}_2 \\ \hline \end{array}$$

RN 859516-41-9 CAPLUS

CN 2-Piperazinecarbonitrile, 1-[[3-[2-[[2-(3,5-difluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 859516-42-0 CAPLUS

CN 2-Pyrimidinamine, 4-[3-[(2,2-dimethyl-1-piperazinyl)methyl]phenyl]-N-[2-(3-fluorophenyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} HN & N \\ \hline N & NH-CH_2-CH_2 \\ \hline Me & Me \\ \end{array}$$

RN 859516-43-1 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[(2,2-dimethyl-1-piperazinyl)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859516-44-2 CAPLUS

CN Phenol, 4-[2-[[4-[3-[(2,2-dimethyl-1-piperazinyl)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859516-45-3 CAPLUS

CN Phenol, 4-[2-[[4-[3-[(3,5-dimethyl-1-piperazinyl)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Me} & \text{N} & \text{CH}_2 & \text{CH}_2 \\ \hline & \text{N} & \text{NH} - \text{CH}_2 - \text{CH}_2 \\ \hline & \text{Me} \end{array}$$

RN 859516-46-4 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[(3,5-dimethyl-1-piperazinyl)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Me N
$$CH_2$$
 N NH CH_2 CH_2 OH N

RN 859516-47-5 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[(3,5-dimethyl-1-piperazinyl)methyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{HN} \\ \text{N} \\ \text{CH}_2 \\ \text{N} \\ \text{NH} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{F} \\ \end{array}$$

RN 859516-48-6 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-(2,5-diazabicyclo[2.2.1]hept-2-ylmethyl)phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859516-49-7 CAPLUS

CN Phenol, 4-[2-[[4-[3-(2,5-diazabicyclo[2.2.1]hept-2-ylmethyl)phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$N$$
 CH_2 N NH CH_2 CH_2 OH

RN 859516-50-0 CAPLUS

CN 2-Pyrimidinamine, 4-[3-(2,5-diazabicyclo[2.2.1]hept-2-ylmethyl)phenyl]-N-[2-(3-fluorophenyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 859516-51-1 CAPLUS

CN 2-Pyrimidinamine, 4-[3-(2,5-diazabicyclo[2.2.1]hept-2-ylmethyl)phenyl]-N-[2-(3,5-difluorophenyl)ethyl]- (9CI) (CA INDEX NAME)

RN 859516-52-2 CAPLUS

CN 2-Pyrimidinamine, 4-[3-(2,5-diazabicyclo[2.2.1]hept-2-ylmethyl)phenyl]-N-[2-(3,5-difluorophenyl)ethyl-2,2-d2]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ &$$

RN 859516-53-3 CAPLUS

CN Phenol, 4-[2-[[4-[3-[(tetrahydro-1,1-dioxido-1,2,5-thiadiazepin-2(3H)-yl)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859516-54-4 CAPLUS

CN Phenol, 4-[2-[[4-[2-methoxy-5-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859516-55-5 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[2-methoxy-5-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859516-59-9 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-methyl-6-[3-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859516-60-2 CAPLUS

CN Piperazine, 1-[[3-[2-[[2-(3,5-difluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]sulfonyl]-2-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 859516-61-3P 859516-62-4P 859516-63-5P 859516-64-6P 859516-65-7P 859516-66-8P 859516-67-9P 859516-68-0P 859516-69-1P 859516-71-5P 859516-73-7P 859516-74-8P 859516-75-9P 859516-76-0P 859518-37-9P 859518-38-0P 859518-39-1P 859518-40-4P 859518-42-6P 859518-44-8P 859518-45-9P 859518-46-0P 859518-47-1P 859518-48-2P 859518-49-3P 859518-50-6P 859518-51-7P 859518-52-8P 859518-53-9P 859518-54-0P

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859518-55-1P 859518-56-2P 859518-57-3P
859518-58-4P 859518-59-5P 859518-60-8P
859518-61-9P 859518-63-1P 859518-64-2P
859518-65-3P 859518-66-4P 859518-67-5P
859518-68-6P 859518-69-7P 859518-70-0P
859518-71-1P 859518-72-2P 859518-73-3P
859518-74-4P 859518-75-5P 859518-76-6P
859518-78-8P 859518-79-9P 859518-80-2P
859518-81-3P 859518-82-4P 859518-83-5P
859518-84-6P 859518-85-7P 859518-86-8P
859518-87-9P 859518-88-0P 859518-89-1P
859518-90-4P 859518-92-6P 859518-93-7P
859518-94-8P 859518-96-0P 859518-97-1P
859518-98-2P 859518-99-3P 859519-00-9P
859519-01-0P 859519-02-1P 859519-03-2P
859519-04-3P 859519-06-5P 859519-07-6P
859519-08-7P 859519-09-8P 859519-10-1P
859519-11-2P 859519-12-3P 859519-13-4P
859519-14-5P 859519-15-6P 859519-16-7P
859519-17-8P 859519-18-9P 859519-19-0P
859519-20-3P 859519-21-4P 859519-22-5P
859519-23-6P 859519-24-7P 859519-25-8P
859519-26-9P 859519-27-0P 859519-28-1P
859519-29-2P 859519-30-5P 859519-31-6P
859519-33-8P 859519-34-9P 859519-35-0P
859519-36-1P 859519-37-2P 859519-38-3P
859519-40-7P 859519-41-8P 859519-42-9P
859519-43-0P 859519-44-1P 859519-45-2P
859519-46-3P 859519-47-4P 859519-48-5P
859519-49-6P 859519-50-9P 859519-51-0P
859519-52-1P 859519-53-2P 859519-54-3P
859519-55-4P 859519-56-5P 859519-57-6P
859519-58-7P 859519-59-8P 859519-60-1P
859519-61-2P 859519-62-3P 859519-63-4P
859519-64-5P 859519-65-6P 859519-66-7P
859519-67-8P 859519-68-9P 859519-69-0P
859519-70-3P 859519-71-4P 859708-81-9P
859708-86-4P 859708-88-6P 859708-91-1P
859708-93-3P 859708-95-5P 859708-97-7P
859708-99-9P 859709-01-6P 859709-04-9P
859709-07-2P 859712-89-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (preparation of aryl pyrimidines as protein kinase C inhibitors)
859516-61-3 CAPLUS
Piperazine, 1-[[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-
pyrimidinyl]phenyl]sulfonyl]-2-methyl-, (2S)- (9CI) (CA INDEX NAME)
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Absolute stereochemistry.

RN

CN

RN 859516-62-4 CAPLUS

CN Piperazine, 1-[[3-[2-[[2-(3-fluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]sulfonyl]-2-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859516-63-5 CAPLUS

CN Piperazine, 1-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]sulfonyl]-2-methyl-, (2S)- (9CI) (CA INDEX NAME)

RN 859516-64-6 CAPLUS

CN Phenol, 4-[2-[[4-[2-methyl-5-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859516-65-7 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[2-methyl-5-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859516-66-8 CAPLUS

CN Phenol, 4-[2-[[4-[2-methyl-3-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859516-67-9 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[4-fluoro-3-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859516-68-0 CAPLUS

CN Phenol, 4-[2-[[4-[4-fluoro-3-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859516-69-1 CAPLUS

CN 2-Pyrimidinamine, 4-[4-fluoro-3-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]-N-[2-(3-fluorophenyl)ethyl]- (9CI) (CA INDEX NAME)

RN 859516-71-5 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[[ethyl[2-(2-piperidinyl)ethyl]amino]methyl]p henyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{C1} & \text{OH} \\ \hline & \text{NH} & \text{CH}_2 - \text{CH}_2 - \text{NH} - \text{CH}_2 - \text{CH}_2 \\ \hline & \text{NH} - \text{CH}_2 - \text{CH}_2 \\ \hline \end{array}$$

RN 859516-73-7 CAPLUS

CN 2-Pyrimidinamine, 4-[3-[[ethyl[2-(2-piperidinyl)ethyl]amino]methyl]phenyl]-N-[2-(3-fluorophenyl)ethyl]- (9CI) (CA INDEX NAME)

RN 859516-74-8 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[[[2-(2-pyridinyl)ethyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \mathsf{CH}_2 - \mathsf{CH}_2 - \mathsf{NH} & \mathsf{N} \\ \mathsf{HO} & \mathsf{C1} \end{array}$$

RN 859516-75-9 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[[[2-(3-pyridinyl)ethyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859516-76-0 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[[[2-(4-pyridinyl)ethyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

HO
$$CH_2-CH_2-NH$$
 $CH_2-NH-CH_2-CH_2$

RN 859518-37-9 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[[ethyl(3S)-3-pyrrolidinylamino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859518-38-0 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[5-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859518-39-1 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-[[ethyl(3R)-3-pyrrolidinylamino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859518-40-4 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[5-[[(2R,5S)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859518-42-6 CAPLUS

CN Phenol, 4-[2-[[4-[3-[(ethyl-4-piperidinylamino)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{HN} & \text{Et} \\ \hline & \text{N} - \text{CH}_2 \\ \hline & \text{N} \\ \end{array}$$

RN 859518-44-8 CAPLUS

CN Phenol, 2-chloro-4-[2-[[4-[3-(1-piperazinylmethyl)phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859518-45-9 CAPLUS

CN Phenol, 4-[2-[[4-[2-fluoro-5-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859518-46-0 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859518-47-1 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[ethyl(3S)-3-pyrrolidinylamino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859518-48-2 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[ethyl(3R)-3-pyrrolidinylamino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859518-49-3 CAPLUS

CN Phenol, 3-[2-[[4-[3-[(ethyl-4-piperidinylamino)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{HN} & \text{Et} \\ \hline & \text{N} - \text{CH}_2 \\ \hline & \text{NH} - \text{CH}_2 - \text{CH}_2 \\ \hline \end{array}$$

RN 859518-50-6 CAPLUS

CN Phenol, 3-[2-[[4-[3-[[ethyl(3S)-3-pyrrolidinylamino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859518-51-7 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[ethyl[(3R)-3-piperidinylmethyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859518-52-8 CAPLUS

CN Phenol, 3-[2-[[4-[5-[[(2R,5S)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859518-53-9 CAPLUS

CN Phenol, 3-[2-[[4-[2-fluoro-5-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859518-54-0 CAPLUS

CN Phenol, 3-[2-[[4-[3-[[ethyl[(3S)-3-piperidinylmethyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859518-55-1 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[ethyl[(2S)-2-pyrrolidinylmethyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859518-56-2 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[ethyl[(3S)-3-pyrrolidinylmethyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859518-57-3 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[cyclopropyl(1-methyl-4-piperidinyl)amino]methyl]phen yl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Me \\ \hline \\ N \\ \hline \\ N \\ CH_2 \\ \hline \\ N \\ NH \\ CH_2 \\ CH_2 \\ \hline \\ OH \\ \end{array}$$

RN 859518-58-4 CAPLUS

CN Phenol, 4-[2-[[4-[5-[[(2R,5S)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859518-59-5 CAPLUS

CN Phenol, 3-[2-[[4-[3-[[ethyl[(3R)-3-pyrrolidinylmethyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859518-60-8 CAPLUS

CN Phenol, 3-[2-[[4-[3-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859518-61-9 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[2-(aminomethyl)-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \mathsf{HN} & \mathsf{CH_2} - \mathsf{NH_2} \\ \mathsf{N} & \mathsf{CH_2} - \mathsf{CH_2} \end{array} \qquad \begin{array}{c} \mathsf{OH} \\ \mathsf{N} & \mathsf{NH} - \mathsf{CH_2} - \mathsf{CH_2} \end{array}$$

RN 859518-63-1 CAPLUS

CN Butanoic acid, 2-amino-4-[ethyl[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859518-64-2 CAPLUS

CN Phenol, 3-[2-[[4-[3-[[ethyl[(3S)-3-pyrrolidinylmethyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859518-65-3 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[ethyl[(2R)-2-pyrrolidinylmethyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859518-66-4 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-[(2S)-2-pyrrolidinylmethyl]- (9CI) (CA INDEX NAME)

RN 859518-67-5 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[((3R,4R)-3-methyl-4-piperidinyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859518-68-6 CAPLUS

CN Phenol, 4-[2-[[4-[3-(1-piperazinylmethyl)phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{HN} & \text{N} \\ \text{N} & \text{CH}_2 \\ \end{array} \begin{array}{c} \text{OH} \\ \text{N} & \text{NH} \\ \end{array}$$

RN 859518-69-7 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[5-[[(2R,5R)-2,5-

dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859518-70-0 CAPLUS

CN Phenol, 3-[2-[[4-[5-[[ethyl[(3S)-3-piperidinylmethyl]amino]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859518-71-1 CAPLUS

CN 2-Pyrimidinamine, 4-[3-[[ethyl[2-(2R)-2-pyrrolidinylethyl]amino]methyl]phe nyl]-N-(2-phenylethyl)- (9CI) (CA INDEX NAME)

RN

859518-72-2 CAPLUS
Phenol, 4-[2-[[4-[5-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]-2-methylphenyl]-2-pyrimidinyl]amino]ethyl]-, rel- (9CI) (CA INDEX NAME) CN

Relative stereochemistry.

RN859518-73-3 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-[4-(acetyloxy)phenyl]ethyl]amino]-4pyrimidinyl]phenyl]methyl]-N-(3-aminopropyl)- (9CI) (CA INDEX NAME)

RN 859518-74-4 CAPLUS

CN Phenol, 4-[2-[[4-[3-[(2,3-dimethyl-1-piperazinyl)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{HN} \end{array} \qquad \text{CH}_2 \qquad \begin{array}{c} \text{OH} \\ \text{N} \end{array} \qquad \text{NH-CH}_2 - \text{CH}_2 \\ \end{array}$$

RN 859518-75-5 CAPLUS

CN Phenol, 3-[2-[[4-[3-[[ethyl[2-(1-piperazinyl)ethyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859518-76-6 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(1S)-2-hydroxy-1-methylethyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859518-78-8 CAPLUS

CN D-Proline, 4-[ethyl[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]amino]-, methyl ester, (4R)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859518-79-9 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[ethyl[(3R)-3-piperidinylmethyl]amino]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859518-80-2 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[ethyl[2-(1-piperazinyl)ethyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \operatorname{HN} & \operatorname{Et} & \operatorname{NH-CH_2-CH_2} & \operatorname{OH} \\ & \operatorname{NH-CH_2-CH_2} & \operatorname{NH-CH_2-CH_2} & \operatorname{OH} \\ \end{array}$$

RN 859518-81-3 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[1-(4-pyridinylmethyl)-4-piperidinyl]amino]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

HO
$$CH_2-CH_2-NH$$
 NH NH CH_2

RN 859518-82-4 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[3-(ethylamino)-8-azabicyclo[3.2.1]oct-8-yl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859518-83-5 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]phenyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859518-84-6 CAPLUS

CN 2-Piperazinepropanoic acid, 4-[[3-[2-[[2-(3-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & \text{HN} & & \\ & \text{N} & \text{CH}_2 \\ & & \text{OH} \\ \end{array}$$

RN 859518-85-7 CAPLUS

CN Phenol, 4-[2-[[4-[5-[(2-ethyl-1-piperazinyl)methyl]-2-methylphenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Et} & \text{OH} \\ \hline & \text{N} & \text{NH-CH}_2\text{--CH}_2 \\ \hline & \text{Me} \end{array}$$

RN 859518-86-8 CAPLUS

CN Phenol, 5-[2-[[4-[5-[[(2R,5S)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]-2-methoxy-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859518-87-9 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[ethyl[(2S)-2-pyrrolidinylmethyl]amino]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859518-88-0 CAPLUS

CN Phenol, 3-[2-[[4-[3-[[3-(ethylamino)-8-azabicyclo[3.2.1]oct-8-yl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859518-89-1 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[2-methoxy-5-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859518-90-4 CAPLUS

CN 2-Piperazinepropanoic acid, 4-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & \text{HN} & \text{N} & \text{CH}_2 \\ & & \text{N} & \text{NH-CH}_2 - \text{CH}_2 \\ \end{array}$$

RN 859518-92-6 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[ethyl[(3S)-3-pyrrolidinylmethyl]amino]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859518-93-7 CAPLUS
CN Phenol, 4-[2-[[4-[3-[(4-amino-1-ethylbutyl)amino]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859518-94-8 CAPLUS
CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[2-fluoro-5-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859518-96-0 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-[2-(2R)-2-pyrrolidinylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859518-97-1 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[ethyl(3S)-3-pyrrolidinylamino]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN

 $859518-98-2 \quad \text{CAPLUS} \\ \text{Phenol, } 3-[2-[[4-[5-[[(2R,5R)-2,5-\text{dimethyl-1-piperazinyl}]\text{methyl}]-2-\text{methylphenyl}]-2-pyrimidinyl]amino]ethyl]-, rel- (9CI) \quad (CA INDEX NAME) \\ \text{CAPLUS} \\ \text{CA$ CN

Relative stereochemistry.

RN859518-99-3 CAPLUS

2-Pyrimidinamine, 4-[3-[[ethyl(3S)-3-pyrrolidinylamino]methyl]phenyl]-N-[2-(3-fluorophenyl)ethyl]- (9CI) (CA INDEX NAME)CN

RN 859519-00-9 CAPLUS

CN 2-Piperazinepropanoic acid, 1-[[3-[2-[[2-(3-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2-\text{CH}_2-\text{CO}_2\text{H} & \text{N} \\ \text{N}-\text{CH}_2-\text{CH}_2-\text{CH}_2 & \text{OH} \\ \end{array}$$

RN 859519-01-0 CAPLUS

CN Phenol, 4-[2-[[4-[4-methyl-3-(4-piperidinylamino)phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{HN} & \text{NH} - \text{CH}_2 - \text{CH}_2 \\ \hline \end{array}$$

RN 859519-02-1 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[ethyl[(3S)-3-piperidinylmethyl]amino]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859519-03-2 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(3,5-difluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-(3S)-3-pyrrolidinyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859519-04-3 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[5-[[ethyl[(3S)-3-piperidinylmethyl]amino]methyl]-2-fluorophenyl]- (9CI) (CA INDEX NAME)

RN 859519-06-5 CAPLUS

CN 2-Piperazinepropanoic acid, 1-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{CH}_2-\text{CH}_2-\text{CO}_2\text{H} & \text{N} \\ \hline \text{N} & \text{NH}-\text{CH}_2-\text{CH}_2 \end{array} \begin{array}{c} \text{OH} \\ \end{array}$$

RN 859519-07-6 CAPLUS

CN 2-Pyrimidinamine, 4-[3-[[ethyl[(2S)-2-pyrrolidinylmethyl]amino]methyl]phen yl]-N-[2-(3-fluorophenyl)ethyl]- (9CI) (CA INDEX NAME)

RN 859519-08-7 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[(2,3-dimethyl-1-piperazinyl)methyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{HN} \\ \text{N} \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{CH}_2 \\ \text{F} \\ \end{array}$$

RN 859519-09-8 CAPLUS

CN Phenol, 2-methoxy-5-[2-[[4-[3-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859519-10-1 CAPLUS

CN 2-Pyrimidinamine, 4-[3-[(ethyl-4-piperidinylamino)methyl]phenyl]-N-[2-(3-methoxyphenyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{HN} & \text{Et} \\ \hline & \text{N} & \text{NH} - \text{CH}_2 - \text{CH}_2 \\ \hline \end{array}$$

RN 859519-11-2 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[ethyl[2-(1-piperazinyl)ethyl]amino]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859519-12-3 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[[2-(2R)-2-pyrrolidinylethyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859519-13-4 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-(1-piperazinylmethyl)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

RN 859519-14-5 CAPLUS

CN 2-Piperazinecarboxylic acid, 4-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$_{\rm HO_2C}$$
 $_{\rm HN}$ $_{\rm N}$ $_{\rm CH_2}$ $_{\rm N}$ $_{\rm NH-CH_2-CH_2}$ $_{\rm CH_2}$

RN 859519-15-6 CAPLUS

CN 2-Pyrimidinamine, 4-[3-[[ethyl(3S)-3-pyrrolidinylamino]methyl]phenyl]-N-[2-(3-methoxyphenyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859519-16-7 CAPLUS

CN Methanesulfonamide, N-(3-aminopropyl)-N-[[3-[6-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

HO
$$CH_2-CH_2-NH$$
 $O=S-Me$ $CH_2-N-(CH_2)_3-NH_2$

RN 859519-17-8 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[ethyl](2R)-2-pyrrolidinylmethyl]amino]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859519-18-9 CAPLUS

CN 2-Piperazinepropanoic acid, 4-[[3-[2-[[2-(3,5-difluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & \text{HN} & & \\ & \text{HO}_2\text{C}-\text{CH}_2-\text{CH}_2 & & \\ & & \text{N} & & \text{NH}-\text{CH}_2-\text{CH}_2 \\ \end{array}$$

RN 859519-19-0 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[[(3R,4R)-3-methyl-4-piperidinyl]amino]methyl]phenyl]-, rel- (9CI) (CA INDEX NAME)

RN 859519-20-3 CAPLUS

CN 2-Pyrimidinamine, 4-[3-[[2-(aminomethyl)-1-piperazinyl]methyl]phenyl]-N-[2-(3-fluorophenyl)ethyl]- (9CI) (CA INDEX NAME)

RN 859519-21-4 CAPLUS

CN 2-Pyrimidinamine, 4-[3-[[ethyl(3R)-3-pyrrolidinylamino]methyl]phenyl]-N-[2-(3-fluorophenyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859519-22-5 CAPLUS

CN Phenol, 3-[2-[[4-[3-[(2,3-dimethyl-1-piperazinyl)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} HN \\ N \\ \hline \\ Me \end{array} \qquad \begin{array}{c} N \\ NH \\ \hline \\ CH_2 \\ \hline \\ OH \end{array} \qquad \begin{array}{c} OH \\ \\ OH \\ \hline \end{array}$$

RN 859519-23-6 CAPLUS

CN 8-Azabicyclo[3.2.1]octan-3-amine, 8-[[3-[2-[[2-(3,5-difluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-ethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ \hline N & & \\ CH_2 & & & \\ \hline N & & \\ NH-CH_2-CH_2 & \\ \hline \end{array}$$

RN 859519-24-7 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[5-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]-2-methylphenyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859519-25-8 CAPLUS

CN 2-Pyrimidinamine, 4-[3-[[2-(aminomethyl)-1-piperazinyl]methyl]phenyl]-N-[2-(3,5-difluorophenyl)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ \text{HN} & & \text{CH}_2 - \text{NH}_2 \\ & & & \text{N} & \text{NH} - \text{CH}_2 - \text{CH}_2 \\ \end{array}$$

RN 859519-26-9 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[(2-ethyl-1-piperazinyl)methyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ &$$

RN 859519-27-0 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(3,5-difluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-[(2S)-2-pyrrolidinylmethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859519-28-1 CAPLUS

CN Phenol, 4-[2-[[4-[3-[(1-propyl-4-piperidinyl)amino]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} n-\text{Pr} & \text{OH} \\ \hline & N \\ \hline & NH-\text{CH}_2-\text{CH}_2 \\ \hline \end{array}$$

RN 859519-29-2 CAPLUS
CN 2-Pyrimidinamine, N-[2-(3-fluorophenyl)ethyl]-4-[3-(1-piperazinylmethyl)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \mathsf{HN} & \mathsf{N} \\ \mathsf{CH_2} & \mathsf{NH} \\ \mathsf{CH_2} - \mathsf{CH_2} \\ \mathsf{F} \end{array}$$

RN 859519-30-5 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(3-fluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-[(2S)-2-pyrrolidinylmethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859519-31-6 CAPLUS

CN Phenol, 3-[2-[[4-[5-[(2-ethyl-1-piperazinyl)methyl]-2-methylphenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{HN} & \text{N} & \text{CH}_2 & \text{CH}_2 \\ \hline & \text{N} & \text{NH} - \text{CH}_2 - \text{CH}_2 \\ \hline & \text{Me} \end{array}$$

RN 859519-33-8 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3-fluorophenyl)ethyl]-4-[3-[(hexahydro-1H-1,4-diazepin-1-yl)methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859519-34-9 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3-fluorophenyl)ethyl]-4-[3-[[[(3R,4R)-3-methyl-4-piperidinyl]amino]methyl]phenyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859519-35-0 CAPLUS

CN Phenol, 4-[2-[[4-[3-[2-(1-pyrrolidinyl)ethoxy]phenyl]-2-pyrimidinyl]amino]ethyl]-, acetate (ester) (9CI) (CA INDEX NAME)

RN 859519-36-1 CAPLUS

CN Methanesulfonamide, N-[[3-[2-[[2-(3,5-difluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-N-[2-(2R)-2-pyrrolidinylethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859519-37-2 CAPLUS

CN 2H-Indol-2-one, 3,3-difluoro-1,3-dihydro-5-[2-[[4-[3-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859519-38-3 CAPLUS

CN 2-Pyrimidinamine, 4-[3-[[ethyl[2-(2R)-2-pyrrolidinylethyl]amino]methyl]phe nyl]-N-[2-(3-fluorophenyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859519-40-7 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[2-methyl-3-[[(2S)-2-methyl-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

RN 859519-41-8 CAPLUS

CN 2-Pyrimidinamine, 4-[3-[[ethyl(3R)-3-pyrrolidinylamino]methyl]phenyl]-N-[2-(3-methoxyphenyl)ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859519-42-9 CAPLUS

CN 2-Piperazinepropanoic acid, 1-[[3-[2-[[2-(3,5-difluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & \text{HN} & & \text{N} \\ & & \text{N} \\ & & \text{CH}_2 \\ & & \text{CH}_2$$

RN 859519-43-0 CAPLUS

CN Phenol, 4-[2-[[2-[3-[[(3-aminopropyl)ethylamino]methyl]phenyl]-5-fluoro-4-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859519-44-1 CAPLUS

CN 1H-Indole-5-ethanamine, 3,7-dichloro-N-[4-[3-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859519-45-2 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[5-[(2-ethyl-1-piperazinyl)methyl]-2-methylphenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 859519-46-3 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(2R,5S)-2-methyl-5-(trifluoromethyl)-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859519-47-4 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]-2-(trifluoromethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859519-48-5 CAPLUS

CN 2-Piperazinecarboxamide, 4-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-5-methyl-, (2R,5S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859519-49-6 CAPLUS

CN 2-Piperazinecarboxamide, 4-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-5-methyl-N-1H-tetrazol-5-yl-, (2R,5R)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859519-50-9 CAPLUS

CN 2-Piperazinecarboxamide, 4-[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-5-methyl-N-1H-tetrazol-5-yl-, (2R,5S)-rel-(9CI) (CA INDEX NAME)

RN 859519-51-0 CAPLUS

CN Phenol, 2-(1,1-dimethylethyl)-4-[2-[[4-[3-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859519-52-1 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]-2-(1-methylethyl)-, rel-(9CI) (CA INDEX NAME)

RN 859519-53-2 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]-2-ethyl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859519-54-3 CAPLUS

CN Phenol, 5-[2-[[4-[3-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]-2-(methylsulfinyl)-, rel-(9CI) (CA INDEX NAME)

RN 859519-55-4 CAPLUS

CN Phenol, 5-[2-[[4-[3-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]-2-(methylsulfonyl)-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859519-56-5 CAPLUS

CN Sulfamic acid, 4-[2-[[4-[3-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]-2-hydroxyphenyl ester, rel- (9CI) (CA INDEX NAME)

RN 859519-57-6 CAPLUS
CN Sulfamic acid, 5-[2-[[4-[3-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]-2-hydroxyphenyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859519-58-7 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]-2-(methylsulfonyl)-, rel- (9CI) (CA INDEX NAME)

RN 859519-59-8 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]-2-(methylsulfinyl)-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859519-60-1 CAPLUS

CN Benzenesulfonamide, 4-[2-[[4-[3-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]-2-hydroxy-, rel-(9CI) (CA INDEX NAME)

RN 859519-61-2 CAPLUS
CN Benzenesulfonamide, 5-[2-[[4-[3-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]-2-hydroxy-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859519-62-3 CAPLUS
CN Benzenesulfinamide, 4-[2-[[4-[5-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]-2-hydroxy-, rel- (9CI) (CA INDEX NAME)

RN 859519-63-4 CAPLUS

CN Phenol, 5-[2-[[4-[5-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]-2-(methylsulfinyl)-, rel-(9CI)(CA INDEX NAME)

Relative stereochemistry.

RN 859519-64-5 CAPLUS

CN Phenol, 5-[2-[[4-[5-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]-2-(methylsulfonyl)-, rel- (9CI) (CA INDEX NAME)

RN 859519-65-6 CAPLUS

CN Sulfamic acid, 4-[2-[[4-[5-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]-2-hydroxyphenyl ester, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859519-66-7 CAPLUS

CN Sulfamic acid, 5-[2-[[4-[5-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]-2-hydroxyphenyl ester, rel- (9CI) (CA INDEX NAME)

RN 859519-67-8 CAPLUS
CN Benzenesulfinamide, 5-[2-[[4-[5-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]-2-hydroxy-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859519-68-9 CAPLUS
CN Phenol, 4-[2-[[4-[5-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]-2-(methylsulfonyl)-, rel-(9CI)(CA INDEX NAME)

Relative stereochemistry.

RN 859519-69-0 CAPLUS
CN Phenol, 4-[2-[[4-[5-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]-2-(methylsulfinyl)-, rel-(9CI)(CA INDEX NAME)

Relative stereochemistry.

RN 859519-70-3 CAPLUS
CN Benzenesulfonamide, 4-[2-[[4-[5-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]-2-hydroxy-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859519-71-4 CAPLUS

CN Benzenesulfonamide, 5-[2-[[4-[5-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]-2-hydroxy-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 859708-81-9 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(2S)-2-methyl-1-piperidinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859708-86-4 CAPLUS

CN Phenol, 4-[2-[[4-[5-[[(2S,5S)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859708-88-6 CAPLUS

CN Phenol, 4-[2-[[4-[5-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859708-91-1 CAPLUS

CN Phenol, 3-[2-[[4-[5-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859708-93-3 CAPLUS

CN Phenol, 3-[2-[[4-[5-[[(2S,5S)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859708-95-5 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[ethyl[(3R)-3-pyrrolidinylmethyl]amino]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859708-97-7 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(2S,5R)-2,5-dimethyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859708-99-9 CAPLUS

CN Phenol, 4-[2-[[4-[3-[[(2R,5S)-2,5-dimethyl-1-piperazinyl]methyl]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859709-01-6 CAPLUS

CN Phenol, 5-[2-[[4-[5-[[(2S,5S)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]-2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859709-04-9 CAPLUS

CN Phenol, 5-[2-[[4-[5-[[(2R,5R)-2,5-dimethyl-1-piperazinyl]methyl]-2-fluorophenyl]-2-pyrimidinyl]amino]ethyl]-2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859709-07-2 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[(2S,5R)-2,5-dimethyl-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859712-89-3 CAPLUS

CN 2-Pyrimidinamine, N-[2-(3,5-difluorophenyl)ethyl]-4-[3-[[(2R,5S)-2,5-dimethyl-1-piperazinyl]methyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

B59516-87-3P 859517-02-5P 859517-03-6P
859517-05-8P, 4-[2-[4-(3-(Dimethoxymethyl)-phenyl)pyrimidin-2ylamino]ethyl]phenol 859517-06-9P 859517-17-2P,
1-(3-[2-[[2-(4-Methoxyphenyl)ethyl]amino]pyrimidin-4-yl]phenyl)ethanone
859517-31-0P 859517-35-4P 859517-36-5P
859517-38-7P 859517-40-1P 859517-47-8P
859517-55-8P 859517-82-1P 859517-83-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

$$_{\rm N}$$
 $_{\rm N}$ $_{\rm NH-CH_2-CH_2}$ $_{\rm OH}$

RN 859517-03-6 CAPLUS
CN Phenol, 4-[2-[[4-[3-[(3-pyridinylmethyl)amino]phenyl]-2-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RN 859517-06-9 CAPLUS

CN Benzaldehyde, 3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 859517-17-2 CAPLUS

CN Ethanone, 1-[3-[2-[[2-(4-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Ac} & \text{N} & \text{NH-CH}_2\text{-CH}_2 \\ \hline \end{array}$$

RN 859517-31-0 CAPLUS

CN Ethanone, 1-[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]-(9CI) (CA INDEX NAME)

RN 859517-35-4 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-[[ethyl[[3-[2-[[2-(3-fluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]amino]carbonyl]-, 1,1-dimethylethyl ester, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859517-36-5 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-[[ethyl[[3-[2-[[2-(3-fluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]amino]carbonyl]-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859517-38-7 CAPLUS

CN 1-Piperazinecarboxylic acid, 4-[[3-[2-[[2-(3-fluorophenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-3-methyl-, 1,1-dimethylethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 859517-40-1 CAPLUS

CN Carbamic acid, [[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl](1-methylethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$t-BuO-C$$
 $i-Pr-N-CH_2$
 N
 $NH-CH_2-CH_2$
OH

RN 859517-47-8 CAPLUS

CN 1-Piperidinecarboxylic acid, 4-[2-[3-[5-fluoro-2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A

O

$$CH_2-CH_2-NH$$
 N
 CH_2-CH_2
 CH_2-CH_2
 N
 CH_2-CH_2

PAGE 1-B

--- OBu-t

RN 859517-55-8 CAPLUS

CN Phenol, 4-[2-[[4-[3-[(ethyl-4-piperidinylamino)methyl]phenyl]-2-pyrimidinyl]amino]ethyl]-2-fluoro- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{HN} & \text{Et} \\ \hline & \text{N} \\ \hline & \text{N} \\ \end{array} \begin{array}{c} \text{CH}_2 \\ \hline \end{array} \begin{array}{c} \text{OH} \\ \end{array}$$

RN 859517-82-1 CAPLUS

CN Carbamic acid, (1,1-dimethylethyl)[[3-[2-[[2-(4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl]-, 2-propenyl ester (9CI) (CA INDEX NAME)

RN 859517-83-2 CAPLUS

CN Carbamic acid, [[3-[2-[[2-(3-chloro-4-hydroxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]methyl](1,1-dimethylethyl)-, 2-propenyl ester (9CI) (CA INDEX NAME)

```
ANSWER 18 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2005:395285 CAPLUS
DN
     142:430294
ΤI
     Preparation of pyrimidine compounds as antistress agents
     Ohmoto, Kazuyuki; Kato, Masashi; Katsumata, Seishi; Manako, Junichiro
IN
PA
     Ono Pharmaceutical Co., Ltd., Japan
SO
     PCT Int. Appl., 133 pp.
     CODEN: PIXXD2
DT
     Patent
     Japanese
LA
FAN.CNT 1
                                                APPLICATION NO.
     PATENT NO.
                           KIND
                                                                          DATE
                                                ______
                                   20050506
PΙ
     WO 2005040135
                            A1
                                                WO 2004-JP16056
                                                                          20041022
         W: AE, AG, AL, AM, AT,
                                   ∖AU, AZ, B̈A, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, II, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
              NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
              TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, TE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, GI, CM, GA, GN, GQ, GW, ML, MR, NE,
              SN, TD, TG
PRAI JP 2003-365237
                                   20031024
                            А
     MARPAT 142:430294
AB
     Title compds. I [ring A = (\log) substituted cyclic group; Q =
     (un) substituted alkyl; (un) substituted cyclic group; ring D =
     (un) substituted cyclic group; W = bond, spacer with a principal chain of 1
     to 4 atoms; Y = spacer with a principal chain of 1 to 4 atoms] were prepared
     For example, benzyloxyacetylation of 4-phenyl-2-aminopyrimidine, e.g.,
     prepared from acetophenone in 2 steps, afforded compound II. In MBR
     (mitochondrial benzodiazepine receptor) binding assays, the Ki value of
     compound III was 0.01 µmol/L. Compoounds I are claimed useful for the
     treatment of depression, asthma etc. Formulations are given.
IT
     850925-11-0P 850925-24-5P 850925-25-6P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (preparation of pyrimidine compds. for treatment of depression, asthma etc.)
RN
     850925-11-0 CAPLUS
CN
     Methanesulfonamide, N-[4-[2,5-bis(difluoromethoxy)phenyl]-2-pyrimidinyl]-N-
     (phenylmethyl) - (9CI) (CA INDEX NAME)
```

RN 850925-24-5 CAPLUS

CN 2-Pyrimidinamine, 4-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-N-methyl-N-

(phenylmethyl) - (9CI) (CA INDEX NAME)

RN 850925-25-6 CAPLUS

CN 2-Pyrimidinamine, 4-[2,5-bis(2,2,2-trifluoroethoxy)phenyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RE.CNT 116 THERE ARE 116 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L10 ANSWER 19 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
AN
      2005:394833 CAPLUS
DN
      142:447114
      A preparation of (indol-1-yl)acetate derivatives, useful as PPAR
ΤI
      Ackermann, Jean; Aebi, Johannes; Binggeli, Alfred; Grether, Uwe; Hirth,
IN
      Georges; Kuhn, Bernd; Maerki, Hans-Peter; Meyer, Markus; Mohr, Peter;
      Wright, Matthew Blake
PA
      Hoffmann-La Roche Inc., USA
      U.S. Pat. Appl. Publ., 39 pp.
SO
      CODEN: USXXCO
DT
      Patent
      English
LΑ
FAN.CNT 1
                                                                                       DATE
                                 KIND
                                           DATE
                                                           APPLICATION NO.
      PATENT NO.
                                 ____
                                          20050505
                                                           US 2004-978144
                                                                                          20041029
PΙ
      US 2005096353
                                   A1
      US 6995263
                                   В2
                                           20060207
                                                           WO 2004-EP12197
                                                                                          20041028
      WO 2005049606
                                  A1
                                           20050602
               AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, BE, BK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TT, TM, TD, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
           TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TT, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
SI, SK, TR, BF, BT, CF, CG, EI, CM, GA, GN, GQ, GW, ML, MR, NE,
                 SN, TD, TG
                                           20031105
PRAI EP 2003-104083
                                   Α
      CASREACT 142:447114; MARPAT 142:447114
OS
      The invention relates to a preparation of (indol-1-yl) acetate derivs.
AΒ
      R10C(O)CH(R2)(R3)R4 [wherein: R1, R2, and R3 are independently selected
       from H or alkyl; R4 is a derivative of indol-1-yl], useful as PPAR activators.
       For instance, (indol-1-yl)acetate I [IC50 (\mumol/L): PPAR\alpha - 1.32,
       PPAR\gamma - >10, PPAR\delta - 0.083] was prepared via etherification of
       Et (5-hydroxyindol-1-yl)acetate by (chloromethyl)pyrimidine derivative II and
       subsequent hydrolysis.
       851069-70-0P, (5-[Methyl-[4-methyl-2-(4-
IT
       trifluoromethylphenyl)pyrimidin-5-ylmethyl]amino]indol-1-yl)acetic acid
       RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
       (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
       (Uses)
           (preparation of (indol-1-yl)acetate derivs. useful as PPAR activators)
       851069-70-0 CAPLUS
RN
       1H-Indole-1-acetic acid, 5-[methyl[[4-methyl-2-[4-(trifluoromethyl)phenyl]-
CN
       5-pyrimidinyl]methyl]amino]- (9CI) (CA INDEX NAME)
```

$$_{\mathrm{F_{3}C}}$$
 $_{\mathrm{N}}$ $_{\mathrm{CH_{2}-N}}$ $_{\mathrm{N}}$ $_{\mathrm{CH_{2}-Co_{2}H}}$

IT **851069-76-6P**, (5-[Methyl-[4-methyl-2-(4-

trifluoromethylphenyl)pyrimidin-5-ylmethyl]amino]indol-1-yl)acetic acid methyl ester

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of (indol-1-yl)acetate derivs. useful as PPAR activators)

RN 851069-76-6 CAPLUS

CN 1H-Indole-1-acetic acid, 5-[methyl[[4-methyl-2-[4-(trifluoromethyl)phenyl]-5-pyrimidinyl]methyl]amino]-, methyl ester (9CI) (CA INDEX NAME)

$$\mathsf{F}_3\mathsf{C} \\ \\ \mathsf{N} \\ \\ \mathsf{CH}_2 \\ \\ \mathsf{N} \\ \\ \mathsf{CH}_2 \\ \\ \mathsf{C} \\$$

RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 20 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
L10
AN
     2005:394829 CAPLUS
     142:463605
DN
     Preparation aryloxyacetic acids and related compounds as PPARS and
TI
     PPARα agonists
IN
     Ackermann, Jean; Aebi, Johannes; Binggeli, Alfred; Grether, Uwe; Hirth,
     Georges; Kuhn, Bernd; Maerki, Hans-Peter; Meyer, Markus; Mohr, Peter;
     Wright, Matthew Blake
PA
     Switz.
     U.S. Pat. Appl. Publ., 89 pp.
SO
     CODEN: USXXCO
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                           KIND
                                  DATE
                                               APPLICATION NO.
                                                                        DATE
                                               -----
                                  20050505
ΡI
     US 2005096337
                            A1 4
                                               US 2004-978155
                                                                        20041029
     AU 2004291262
                            Α1
                                  20050602
                                               AU 2004-291262
                                                                        20041028
     WO 2005049573
                                  20050602
                                               WO 2004-EP12217
                            A1
                                                                        20041028
         W: AE, AG, AL, AM, AT, AU, AZ
                                           BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
              NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
              TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
              EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
              SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
              SN, TD, TG
PRAI EP 2003-104081
                                  20031105
                            Α
     EP 2004-100759
                                  20040226
                            Α
     WO 2004-EP12217
                            W
                                  20041028
os
     MARPAT 142:463605
     Title compds. I [X = O, S, CH2; R1 = H, alkyl; R2 = H, alkyl with
AΒ
     provisos; R3 = H, alkyl; R4, R8 = H, alkyl, cycloalkyl, etc.; R5, R6, R7 =
     H, alkyl, cycloalkyl, etc.] and their pharmaceutically acceptable salts
     and formulations were prepared For example, saponification of Et ester II (Z =
     OEt), afforded acid II (Z = OH) as a light yellow solid. In PPAR\alpha
     receptor binding assays, 3-examples of compds. I exhibited IC50 values
     ranging from 0.013-0.289 \mu mmol/l . Compds. I are claimed to be useful
     for the treatment of diseases modulated by PPAR\delta and PPAR\alpha
     agonist.
IT
     851506-16-6P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
         (preparation aryloxyacetic acids and related compds. as PPAR8 and
        PPARα agonists)
RN
     851506-16-6 CAPLUS
CN
     Acetic acid, [4-[[[4-cyclopropyl-2-[4-(trifluoromethyl)phenyl]-5-
```

pyrimidinyl]methyl]methylamino]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

IT 851507-63-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation aryloxyacetic acids and related compds. as PPAR $\!\delta$ and PPAR $\!\alpha$ agonists)

RN 851507-63-6 CAPLUS

CN Acetic acid, [4-[[[4-cyclopropyl-2-[4-(trifluoromethyl)phenyl]-5-pyrimidinyl]methyl]methylamino]-2-methylphenoxy]-, methyl ester (9CI) (CA INDEX NAME)

```
ANSWER 21 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
L10
AN
     2005:371230 CAPLUS
DN
     142:430289
ΤI
     Preparation of pyrimidine compounds as mixed lymphocyte reaction (MLR)
     inhibitors
     Tsuruoka, Hiroyuki; Matsuda, Akihisa; Sugano, Yuichi; Tatsuta, Toru
IN
PA
     Sankyo Company, Limited, Japan
SO
     PCT Int. Appl., 350 pp.
     CODEN: PIXXD2
DT
     Patent
LА
     Japanese
FAN.CNT 1
     PATENT NO.
                            KIND
                                    DATE
                                                 APPLICATION NO.
                                                                           DATE
                                   120050428
     WO 2005037801
                                                 WO 2004-JP15955
PΙ
                             A1
                                                                           20041021
         W: AE, AG, AL, AM, AT, AU, AZ,
                                              BA, BB, BG, BR, BW, BY, BZ, CA, CH,
              CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
              GE, GH, GM, HR, HU, LD, LL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
              NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
         TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
              SN, TD, TG
     JP 2005145956
                                    20050609
                                                 JP 2004-302344
                             A2
                                                                           20041018
PRAI JP 2003-360967
                                    20031021
OS
     MARPAT 142:430289
AΒ
     Disclosed is a pyrimidine derivative with excellent MLR inhibitory effect or a
     pharmacol. acceptable salt thereof. Pyrimidine derivs. represented by the
     general formula (I) or pharmacol. acceptable salts thereof [R1 = lower
     alkyl; R2 = each (un) substituted aryl or heterocyclyl; A = NH, O; R3 = H,
     lower alkyl, heterocyclyl, aryl, heterocyclyl, -NHR6 (wherein R6 = lower
     alkyl, cycloalkyl-lower alkyl, aralkyl, each (un)substituted cycloalkyl,
     aryl, or heterocyclyl); R4 = H, lower alkyl, lower alkoxy,
     cycloalkyl-lower alkyl, aralkyl, each (un)substituted aryl or
     heterocyclyl; provided that R3 = R4 \neq H; R5 = H, halo, lower alkyl,
     cycloalkyl, (un)substituted heterocyclyl, NR7R8, OR7 (wherein R7, R8 = H,
     cycloalkyl, (un)substituted aryl or lower alkyl)] are prepared These
     compds. exhibit excellent MLR inhibitory effect and are useful as
     inhibitors of allograft rejection in bone marrow and organ transplant or
     for the prevention and/or treatment of inflammatory diseases,
     organ-specific or organ-nonspecific autoimmune diseases, allergic
     diseases, chronic rheumatism, multiple sclerosis, inflammatory bowel
     disease, diabetes, glomerulonephritis, primary biliary liver cirrhosis,
     chronic active hepatitis, pernicious anemia, chronic thyroiditis, atrophic
     gastritis, myasthenia gravis, psoriasis, Sjoegren's syndrome, systemic
     lupus erythematosus, rhinitis, asthma, or atopic dermatitis. Thus, 0.1
     mmol 4-hydrazino-2,6-bis(2-methoxyphenylamino)pyrimidine was dissolved in
     1 mL ethanol, treated with 0.1 mmol 4-acetylpyridine, and stirred for 18 h \,
     to give 4-[N'-[1-(pyridin-4-yl)ethylidene]hydrazino]-2,6-bis(2-
     methoxyphenylamino)pyrimidine. N-methyl-4-[1-[[5-phenyl-2-phenylamino-6-
     [4-(pyridin-4-yl)pyrazol-1-yl]pyrimidin-4-yl]hydrazono]ethyl]benzenesulfon
     amide (II) inhibited MLR in human peripheral hemolymphocyte offered from
     two healthy people with IC50 of 1.0 ng/mL.
IT
     850757-99-2P 850758-00-8P 850758-01-9P
```

850758-06-4P 850758-07-5P 850758-08-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrimidine compds. as mixed lymphocyte reaction (MLR) inhibitors)

RN 850757-99-2 CAPLUS

CN 4(1H)-Pyrimidinone, 6-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-5-phenyl-2-(phenylamino)-, [1-(4-pyridinyl)ethylidene]hydrazone (9CI) (CA INDEX NAME)

RN 850758-00-8 CAPLUS

CN Benzenesulfonamide, 4-[1-[[6-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-5-phenyl-2-(phenylamino)-4-pyrimidinyl]hydrazono]ethyl]-N-methyl- (9CI) (CA INDEX NAME)

RN 850758-01-9 CAPLUS

CN 4(1H)-Pyrimidinone, 6-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-5-phenyl-2-(phenylamino)-, [1-[4-(methylsulfonyl)phenyl]ethylidene]hydrazone (9CI) (CA INDEX NAME)

RN 850758-06-4 CAPLUS

CN 4(1H)-Pyrimidinone, 6-[{(3,4-dimethoxyphenyl)methyl]amino}-5-phenyl-2-(phenylamino)-, [1-(4-pyridinyl)ethylidene]hydrazone (9CI) (CA INDEX NAME)

RN 850758-07-5 CAPLUS

CN Benzenesulfonamide, 4-[1-[[6-[[(3,4-dimethoxyphenyl)methyl]amino]-5-phenyl-2-(phenylamino)-4-pyrimidinyl]hydrazono]ethyl]-N-methyl- (9CI) (CA INDEX NAME)

RN 850758-08-6 CAPLUS

CN 4(1H)-Pyrimidinone, 6-[[(3,4-dimethoxyphenyl)methyl]amino]-5-phenyl-2-(phenylamino)-, [1-[4-(methylsulfonyl)phenyl]ethylidene]hydrazone (9CI) (CA INDEX NAME)

IT 850760-30-4P 850760-57-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyrimidine compds. as mixed lymphocyte reaction (MLR) inhibitors)

RN 850760-30-4 CAPLUS

CN 4(1H)-Pyrimidinone, 6-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-5-phenyl-2-(phenylamino)-, hydrazone (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{NHPh} & \text{OMe} \\ \hline & \text{N} & \text{N} \\ & \text{H}_2\text{N}-\text{NH} & \text{Ph} \end{array}$$

RN 850760-57-5 CAPLUS

CN 4(1H)-Pyrimidinone, 6-[[(3,4-dimethoxyphenyl)methyl]amino]-5-phenyl-2-(phenylamino)-, hydrazone (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{NHPh} & \text{OMe} \\ \hline & \text{N} & \text{NH-CH}_2 \\ \hline & \text{Ph} \end{array}$$

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/671,070

L10 ANSWER 22 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

2005:340499 CAPLUS AN

DN 142:392564

Preparation of pyridopyrimidine-fused steroids anticoccidial agents via ΤI cyclocondensation

Nagamatsu, Tomofumi IN

PA Okayama University, Japan

Jpn. Kokai Tokkyo Koho, 25 pp. SO

CODEN: JKXXAF

DT Patent

LΑ Japanese

PATENT NO.	KIND	PATE	APPLICATION NO.	DATE
PI JP 2005104868 PRAI JP 2003-337640	A2 /	20050421 20030929	JP 2003-337640	20030929

OS MARPAT 142:392564

Pyridopyrimidine-fused steroids, e.g. of formula I [R1 = H, alkyl; R2 = AΒ alkyl, (substituted) Ph, etc. afe prepared via cyclocondensation. The compds. are useful as anticoccidial agents (no data). Thus, II was prepared from 6-(methylamino)-2-phenyl-4(1H)pyrimidinone and 2-(hydroxymethylene)dihydrotestosterone in 76% yield.

IT 66487-67-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of pyridopyrimidine-fused steroids as anticoccidial agents)

RN 66487-67-0 CAPLUS

CN 4(1H)-Pyrimidinone, 2-phenyl-6-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

10/671,070

L10 ANSWER 23 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2005:329965 CAPLUS

DN 143:41343

TI A small-molecule agonist of the Wnt signaling pathway

AU Liu, Jun; Wu, Xu; Mitchell, Brian; Kintner, Chris; Ding, Sheng; Schultz, Peter G.

CS Department of Chemistry and The Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA/ 92037, USA

SO Angewandte Chemie, International Edition (2005), 44(13), 1987-1990 CODEN: ACIEF5; ISSN: 1433-7851

PB Wiley-VCH Verlag GmbH & Co. KGaA

DT Journal

LA English

OS CASREACT 143:41343

AB A new tool for developmental biol.: A screen of combinatorial chemical libraries identified the 2-amino-4,6-disubstituted pyrimidine 1 as a dose-dependent agonist of Wnt signaling. Tadpoles that developed from embryos treated with 1 had substantial head defects (see right-hand image; left=control). Compound 1 appears to mimic the effects of a Wnt ligand in a Xenopus model and may be a useful tool in the study of physiol. processes that involve the Wnt pathway.

IT 853220-52-7P

RL: ADV (Adverse effect, including toxicity); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(identification of substituted pyrimidine compound as small-mol. agonist of Wnt signaling pathway in human cells and Xenopus model)

RN 853220-52-7 CAPLUS

CN 2,4-Pyrimidinediamine, N4-(1,3-benzodioxol-5-ylmethyl)-6-(3-methoxyphenyl)-(9CI) (CA INDEX NAME)

RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 24 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
     2005:300435 CAPLUS
AN
     142:373859
DN
ΤI
     Preparation of pyrimidine and pyridine derivatives useful as HMG-CoA
     reductase inhibitors
IN
     Ahmad, Saleem; Robl, Jeffrey A.; Ngu, Khehyong
PA
     Bristol-Myers Squibb Company, USA
     PCT Int. Appl., 103 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     English
LΑ
FAN.CNT 1
     PATENT NO.
                          KIND
                                 ĎΆΤΕ
                                              APPLICATION NO.
                                                                      DATE
PΙ
     WO 2005030758
                           A1
                                 20050407
                                              WO 2004-US31212
                                                                      20040922
         W: AE, AG, AL, AM, AT, AU, AZ,
                                          ∮BA, BB, BG, BR, BW, BY, BZ, CA, CH,
                                 DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             CN, CO, CR, CU, CZ)
             GE, GH, GM, HR, HU, ID, LL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
         SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
             SN, TD, TG
     US 2005085497
                                 r20050421
                                              ปุ๋ร 2004-946055
                           A1
                                                                      20040921
                                 20060614
                                             ÊP 2004−784885
     EP 1667997
                           A1
                                                                      20040922
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY/, AL, TR, BG, CZ, EE, HU, PL, SK, HR
PRAI US 2003-505893P
                           Ρ
                                 20030925
     WO 2004-US31212
                           W
                                 20040922
     MARPAT 142:373859
OS
     Title compds. I [X = N, CR5; R1=2^{\prime} = H, alkyl, alkoxyalkyl, etc.; R3 =
AB
     (hetero)aryl, cycloalkyl, etc.; R4 = H, (cyclo)alkyl, haloalkyl, etc.; R5
     = H, alkyl; Z = hydroxyalkyl, etc.] are prepared For instance, II is prepared
     in 5 steps from a substituted pyrimidine, 2-methyl-2H-[1,2,4]triazol-3-
     ylamine, and a prior art homochiral dihydroxy acetonide derivative I are
     HMG-CoA reductase inhibitors and are active in inhibiting cholesterol
     biosynthesis, modulating blood serum lipids, for example, lowering LDL
     cholesterol and/or increasing HDL cholesterol, and treating
     hyperlipidemia, dyslipidemia, hormone replacement therapy,
     hypercholesterolemia, hypertriglyceridemia and atherosclerosis as well as
     Alzheimer's disease and osteoporosis [no data].
IT
     849469-56-3P 849470-51-5P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of pyrimidine and pyridine derivs. useful as HMG-CoA reductase
        inhibitors)
RN
     849469-56-3 CAPLUS
CN
     6-Heptenoic acid, 7-[4-(4-fluorophenyl)-2-[[(4-methoxyphenyl)methyl](1-
     methyl-1H-pyrazol-5-yl)amino]-6-(1-methylethyl)-5-pyrimidinyl]-3,5-
     dihydroxy-, monosodium salt, (3R,5S,6E)- (9CI) (CA INDEX NAME)
```

Absolute stereochemistry.
Double bond geometry as shown.

Na

RN 849470-51-5 CAPLUS

CN 6-Heptenoic acid, 7-[4-(4-fluorophenyl)-2-[[(4-methoxyphenyl)methyl](1-methyl-1H-pyrazol-5-yl)amino]-6-(1-methylethyl)-5-pyrimidinyl]-3,5-dihydroxy-, (3R,5S,6E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

IT 849470-74-2P 849470-76-4P 849470-78-6P 849470-80-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyrimidine and pyridine derivs. useful as HMG-CoA reductase inhibitors)

RN 849470-74-2 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-fluorophenyl)-2-[[(4-methoxyphenyl)methyl](1-methyl-1H-pyrazol-5-yl)amino]-6-(1-methylethyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 849470-76-4 CAPLUS

CN 5-Pyrimidinemethanol, 4-(4-fluorophenyl)-2-[[(4-methoxyphenyl)methyl](1-methyl-1H-pyrazol-5-yl)amino]-6-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 849470-78-6 CAPLUS

CN 5-Pyrimidinecarboxaldehyde, 4-(4-fluorophenyl)-2-[[(4-methoxyphenyl)methyl](1-methyl-1H-pyrazol-5-yl)amino]-6-(1-methylethyl)-(9CI) (CA INDEX NAME)

RN 849470-80-0 CAPLUS

CN 2H-Pyran-2-one, 6-[(1E)-2-[4-(4-fluorophenyl)-2-[[(4-methoxyphenyl)methyl](1-methyl-1H-pyrazol-5-yl)amino]-6-(1-methylethyl)-5-pyrimidinyl]ethenyl]tetrahydro-4-hydroxy-, (4S,6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 25 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
      2005:260034 CAPLUS
AN
DN
      142:336376
      Preparation of pharmaceutically active 4,6-disubstituted aminopyrimidine
TI
     derivatives as modulators of protein kinases
     Choidas, Axel; Backes, Alexander; Cotten, Matt; Engkvist, Ola; Felber,
IN
     Beatrice; Freisleben, Achim; Godl, Klaus; Greff, Zoltan; Habenberger,
     Peter; Hafenbradl, Doris; Hartung, Christian; Herget, Thomas; Hoppe,
     Edmund; Klebl, Bert; Missio, Andrea; Mueller, Gerhard; Schwab, Wilfried;
      Zech, Birgit; Bravo, Jose; Harris, John; Le, Joelle; Macritchie, Jackie;
      Savic, Vladimir; Sherborne, Brad; Simpson, Don; Simpson, Don
     Axxima Pharmaceuticals AG, Germany
PA
SO
     PCT Int. Appl., 211 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                             KIND
                                     DATE
                                                   APPLICATION NO.
                                                                               DATE
                                                    ______
                             ____
     WO 2005026129
                                     20050324
                                                   WO 2004-EP10353
PΙ
                              A1
                                                                               20040915
          W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
               CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
          NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
               SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
               SN, TD, TG
PRAI EP 2003-20888
                              Α
                                     20030915
     US 2003-504527P
                              Ρ
                                     --- 20030922
     EP 2004-10308
                              Α
                                     20040430
     US 2004-569806P
                              Ρ
                                     20040512
os
     MARPAT 142:336376
AB
     The invention is related to the preparation of title compds. I, and/or
     stereoisomeric forms and/or pharmaceutically acceptable salts [wherein R1
     = H, (un)substituted alk(en/yn)yl; R2, R4 = independently H, F, Cl, Br, I,
     CN, NH2, NO2, (un) substituted alk(en/yn)yl; R3 = F, Cl, Br, I,
      (un) substituted hetero/aryl, etc.; X = R5-[LR6]m; R5 = (un) substituted
     hetero/aryl, heterocyclyl, cycloalkyl, etc.; R6 = H, (un)substituted
     alkyl, hetero/aryl, heterocyclyl, etc.; L = NRSO2, NRSO; R = H,
      (un) substituted alkyl, SO2-alkyl, etc.] as protein kinase inhibitors for
     use in the prophylaxis and/or treatment of infectious diseases, including
     opportunistic diseases, prion diseases, immunol. diseases, autoimmune
     diseases, bipolar and clin. disorders, cardiovascular diseases, cell
     proliferative diseases, diabetes, inflammation, transplant rejections,
     erectile dysfunction, neurodegenerative diseases and stroke. The
```

invention is also related to a medium comprising at least one of compds. I

General preparation procedures and 5 individual synthetic examples are given.

in an immobilized form and its use for enriching, purifying and/or depleting nucleotide binding proteins which bind to the immobilized I.

I have an inhibitory effect on the protein kinase activity of various protein kinases, such as Abl, CDK1, CDK5, etc. Selected I had an

inhibitory effect on CDK9 and CDK2 with IC50 values in the range of 1 to 1000 nM. I were potent inhibitors of HIV and HCMV replication in cell cultures; for example II showed inhibition of HCMV replication in HFF

cells.

B48638-78-8P, [6-(2-Methoxyphenyl)pyrimidin-4-yl](4phenoxybenzyl)amine 848638-97-1P, 4-[[6-(2Methoxyphenyl)pyrimidin-4-ylamino]methyl]benzenesulfonamide
848639-71-4P, (4-Methylsulfonylbenzyl)[6-(2methoxyphenyl)pyrimidin-4-yl]amine
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

(drug candidate; preparation of 4,6-disubstituted aminopyrimidines as modulators of protein kinases)

RN 848638-78-8 CAPLUS

CN 4-Pyrimidinamine, 6-(2-methoxyphenyl)-N-[(4-phenoxyphenyl)methyl]- (9CI) (CA INDEX NAME)

RN 848638-97-1 CAPLUS

CN Benzenesulfonamide, 4-[[[6-(2-methoxyphenyl)-4-pyrimidinyl]amino]methyl]-(9CI) (CA INDEX NAME)

$$H_2N-S$$
 CH_2-NH
 MeO

RN 848639-71-4 CAPLUS

CN 4-Pyrimidinamine, 6-(2-methoxyphenyl)-N-[[4-(methylsulfonyl)phenyl]methyl]-(9CI) (CA INDEX NAME)

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 26 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
     2005:120896 CAPLUS
AN
DN
     142:198096
TI
     Preparation of 2-acyl-4-amino-5-arylpyrimidines as pesticides and
     fungicides.
IN
     Schwoegler, Anja; Gewehr, Markus; Mueller, Bernd; Grote, Thomas;
     Grammenos, Wassilios; Tormo I. Blasco, Jordi; Gypser, Andreas;
     Rheinheimer, Joachim; Blettner, Carsten; Schaefer, Peter; Schieweck,
     Frank; Wagner, Oliver; Stierl, Reinhard; Schoefl, Ulrich; Strathmann,
     Siegfried; Scherer, Maria
PA
     BASF Aktiengesellschaft, Germany
     PCT Int. Appl., 79 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     German
LΑ
FAN.CNT 2
                                   DATE
     PATENT NO.
                            KIND
                                                 APPLICATION NO.
                                                                           DATE
                                    20050210
                                                 WO 2004-EP7877
PΙ
     WO 2005012261
                             A1
                                                                           20040715
         NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GB, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, GI, CM, GA, GN, GQ, GW, ML, MR, NE,
              SN, TD, TG
                                   20050210
     AU 2004261373
                             A1
                                                 AU 2004-261373
                                                                           20040715
     CA 2532718
                             AA
                                    20050210
                                                 CA 2004-2532718
                                                                           20040715
              AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
     EP 1651618
              IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
PRAI DE 2003-10333857
                             Α
                                    20030724
     DE 2003-10357714
                                    20031209
                             Α
     WO 2004-EP7877
                                    20040715
                             W
OS
     MARPAT 142:198096
AΒ
     Title compds. [I; n = 1-5; L = halo, cyano, cyanato, alkyl, alkenyl,
     alkynyl, alkoxy, alkenyloxy, alkynyloxy, cycloalkyl, cycloalkoxy, etc.;
     R1, R2 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl,
     halocycloalkyl; R1R2N = atoms to form 5-6 membered (substituted)
     heterocyclyl; R3 = halo, cyano, alkyl, alkenyl, alkynyl, cycloalkyl,
     alkoxy, alkenyloxy, alkynyloxy, alkylthio, etc.; R4 = CONHXRa,
     C(ORb):NXRa; X = bond, CO, CONH, CO2, O, imino, etc.; Ra = H, alkyl,
     alkenyl, alkynyl, PhCH2; Rb = H, alkyl, alkenyl, alkynyl], were prepared
     Thus, (S)-4-chloro-6-(2,2,2-trifluoro-1-methylethylamino)-5-(2,4,6-
     trifluorophenyl)pyrimidine-2-carbonitrile was stirred with K2CO3 and H2O2
     in Me2SO at 10°-room temperature to give (S)-4-chloro-6-(2,2,2-trifluoro-
     1-methylethylamino)-5-(2,4,6-trifluorophenyl)pyrimidine-2-carboxamide.
     The latter at 250 ppm on tomatoes gave complete protection against
     Phytophthora infestans.
IT
     838838-75-8P 838838-77-0P
     RL: AGR (Agricultural use); BSU (Biological study, unclassified); BUU
     (Biological use, unclassified); SPN (Synthetic preparation); BIOL
      (Biological study); PREP (Preparation); USES (Uses)
         (preparation of acylaminoarylpyrimidines as pesticides and fungicides)
```

RN 838838-75-8 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-4-fluorophenyl)-6-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
O & NH-CH_2-Ph \\
H_2N-C & N & F \\
N & Cl & Cl & Cl
\end{array}$$

RN 838838-77-0 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,4-difluorophenyl)-6-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & NH-CH_2-Ph \\ H_2N-C & N & F \\ \hline & N & F \\ \hline & C1 & F \\ \end{array}$$

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 27 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
L10
      2005:120774 CAPLUS
AN
DN
      142:194227
ΤI
      Synthesis of 2,4-bis(alkylamino)pyrimidines and their use as
      antimicrobials
      Marquais-Bienewald, Sophie; Hoelzl, Werner; Preuss, Andrea; Mehlin,
IN
      Andreas
PA
      Ciba Specialty Chemicals Holding Inc., Switz.
SO
      PCT Int. Appl., 38 pp.
      CODEN: PIXXD2
DT
      Patent
LА
      English
FAN.CNT 1
      PATENT NO.
                              KIND
                                       ĎAŤE
                                                     APPLICATION NO.
                                                                                  DATE
                                                     _____
                                                                                  _____
                               A2
                                       20050210
PΙ
      WO 2005011758
                                                     WO 2004-EP51516
                                                                                  20040716
      WO 2005011758
                               А3
                                       20050428
               AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, Ch, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
               GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
          NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
               SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
               SN, TD, TG
                                                                                  20040716
   EP 1648524
                               A2
                                       20060426
                                                     EP 2004-766240
               AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
               IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK
PRAI EP 2003-102296
                                       20030725
                               Α
      WO 2004-EP51516
                               W
                                       20040716
OS
      MARPAT 142:194227
AB
      Provided are various 2,4-bis(alkylamino)pyrimidines and their use as
      antimicrobials. The synthesized compds. were demonstrated to have
      antimicrobial activity against bacteria such as Staphylococcus aureus and
      Escherichia coli as well as fungi such as Candida albicans and Aspregillus
      niger. The intended use of these 2,4-bis(alkylamino)pyrimidines are as
      biocides or preservatives in numerous products such as paints, textiles,
      and plastics. Some of the compds. may also find use in cosmetic
      formulations or in mouthwashes.
IT
      838903-20-1 838903-22-3
      RL: BSU (Biological study, unclassified); PRP (Properties); BIOL
      (Biological study)
          (synthesis of 2,4-bis(alkylamino)pyrimidines and their use as
         antimicrobials)
RN
      838903-20-1 CAPLUS
      2,4-Pyrimidinediamine, N2,N2-dimethyl-6-phenyl-N4-(2-phenylethyl)- (9CI)
CN
```

(CA INDEX NAME)

RN 838903-22-3 CAPLUS

CN 2,4-Pyrimidinediamine, N2-octyl-6-phenyl-N4-(2-phenylethyl)- (9CI) (CA INDEX NAME)

IT 838902-75-3P

RL: BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (synthesis of 2,4-bis(alkylamino)pyrimidines and their use as antimicrobials)

RN 838902-75-3 CAPLUS

CN 2,4-Pyrimidinediamine, N2,6-diphenyl-N4-(phenylmethyl)- (9CI) (CA INDEX NAME)

10/671,070

L10 ANSWER 28 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2005:93051 CAPLUS

DN 142:316792

TI Efficient conversion of Biginelli 3,4-dihydropyrimidin-2(1H)-one to pyrimidines via PyBroP-mediated coupling

AU Kang, Fu-An; Kodah, Jason; Guap, Qunying; Li, Xiaobing; Murray, William V.

CS Johnson Johnson Pharmaceutical Research and Development, LLC, Raritan, NJ, 08869, USA

SO Journal of Organic Chemistry (2005), 70(5), 1957-1960 CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

OS CASREACT 142:316792

AB An efficient two-step procedure to convert the Biginelli 3,4-dihydropyrimidin-2(1H)-one to various multifunctionalized pyrimidines, e.g., I, is described. The Biginelli 3,4-dihydropyrimidin-2(1H)-one underwent Kappe dehydrogenation followed by a mild PyBroP-mediated coupling with C, N, O, and S nucleophiles, which provided a readily accessible multifunctionalized pyrimidine template for diversity-oriented synthesis.

IT 848301-51-9P 848301-52-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of pyrimidines via Biginelli reaction of benzaldehyde with malonate and urea followed by Kappe dehydration, and PyBroP-mediated

coupling with nucleophiles) 848301-51-9 CAPLUS

RN 848301-51-9 CAPLUS
CN 5-Pyrimidinecarboxylic acid, 4-methyl-6-phenyl-2-[(phenylmethyl)amino]-,
 methyl ester (9CI) (CA INDEX NAME)

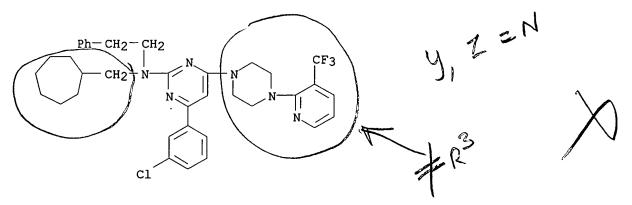
RN 848301-52-0 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-methyl-2-[methyl(phenylmethyl)amino]-6-phenyl-, methyl ester (9CI) (CA INDEX NAME)

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 29 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
L10
AN
     2005:71173 CAPLUS
DN
     142:176866
ΤI
     Preparation of biaryl piperazinyl-pyridine analogues as capsaicin receptor
     modulators
IN
     Bakthavatchalam, Rajagopal; Blum, Charles A.; Brielmann, Harry; Chenard,
     Bertrand L.; De Lombaert, Stephane; Hodgetts, Kevin J.; Hutchison, Alan;
     Yoon, Taeyoung; Zheng, Xiaozhang
     Neurogen Corporation, USA
PA
     PCT Int. Appl., 381 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                           KIND
                                   DATE
                                                APPLICATION NO.
                                                                          DATE
                           ____
                                                -----
ΡI
     WO 2005007648
                            A2
                                   20050127
                                                WO 2004-US23064
                                                                          20040716
     WO 2005007648
                            A3
                                   20050324
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
              CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
              GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
              LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
              NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
         TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
              SN, TD, TG
     AU 2004257289
                                   20050127
                                                AU 2004-257289
                                                                          20040716
                            A1
     CA 2531619
                                   20050127
                                                CA 2004-2531619
                            AA
                                                                          20040716
                                   20060412
                                                EP 2004-778532
                                                                          20040716
     EP 1644358
                            A2
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK
PRAI US 2003-488564P
                            Ρ
                                   20030716
     US 2003-516135P
                            Р
                                   20031031
     WO 2004-US23064
                            W
                                   20040716
     MARPAT 142:176866
os
     The title compds. I [Ar2 = (un)substituted Ph, 6-membered aromatic
AB
     heterocycle; X, Y, Z = CRx, N (at least one of X, Y and Z = N); K, J, F =
     N, CH or carbon substituted with R1; Rx = H, alkyl, NH2, CN, mono or
     dialkylamino; R1 = halo, OH, NH2, CN, etc.; R3 = H, halo, phenylalkyl,
     cycloalkylalkyl, etc.; R4 = H, alkyl, haloalkyl, oxo], useful for treating
     conditions related to capsaicin receptor activation, were prepared E.g., a
     2-step synthesis of II, starting from 2,4,6-trichloropyrimidine and
     morpholine, was given. The compds. I were evaluated for agonist and
     antagonist capsaicin receptor activity (data given). Pharmaceutical
     compns. and methods for using compds. I to treat disorders related to
     capsaicin receptor activation (pain, asthma, etc.), are provided, as are
     methods for using such ligands, for receptor localization studies.
ΙT
     833462-80-9P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
      (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
         (preparation of biaryl piperazinyl-pyridine analogs as capsaicin receptor
         modulators)
RN
     833462-80-9 CAPLUS
CN
     2-Pyrimidinamine, 4-(3-chlorophenyl)-N-(cycloheptylmethyl)-N-(2-
```

phenylethyl)-6-[4-[3-(trifluoromethyl)-2-pyridinyl]-1-piperazinyl]- (9CI)
(CA INDEX NAME)



ANSWER 30 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

L10

```
AN
     2005:29315 CAPLUS
DN
     142:114092
ΤI
     Preparation of pyrimidines as modulators of voltage-gated ion channels
IN
     Wilson, Dean Mitchell; Martinborough, Esther; Neubert, Timothy Donald;
     Termin, Andreas Peter; Gonzales, Jesus E., III; Zimmermann, Nicole
PA
     Vertex Pharmaceuticals Incorporated, USA
SO
     PCT Int. Appl., 195 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
                         KIND
     PATENT NO.
                                DATE
                                             APPLICATION NO.
                                                                     DATE
                         ____
                                             _____
ΡI
     WO 2005003099
                          A2
                                 20050113
                                             WO 2004-US21440
                                                                     20040702
     WO 2005003099
                          Α3
                                 20050512
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
             EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
             SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
             SN, TD, TG
     AU 2004253962
                                 20050113
                                             AU 2004-253962
                          A1
                                                                     20040702
     CA 2531061
                          AΑ
                                 20050113
                                             CA 2004-2531061
                                                                     20040702
     US 2005049247
                          A1
                                 20050303
                                             US 2004-884865
                                                                     20040702
                                             EP 2004-777512
     EP 1638955
                          A2
                                 20060329
                                                                     20040702
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
PRAI US 2003-484362P
                          Ρ
                                 20030702 -
     US 2003-500200P
                          P
                                 20030904
     WO 2004-US21440
                          W
                                 20040702
os
     MARPAT 142:114092
AΒ
     The title compds. [I; R5 = COR3, CO2R3, or R5'; R5' = CONH2 and derivs.,
     SO2H and derivs., CON(CN)H and derivs., etc.; R1, R2 = independently H,
     (un) substituted aliphatic, 5-6-membered aryl ring containing 0-5 heteroatoms,
or
     a 3-7-membered saturated or partially unsatd. ring containing 0-3 heteroatoms;
or
     R1NR2 = (un)substituted 3-8-membered heterocyclyl or heteroaryl containing 1-3
     heteroatoms; A = (un)substituted 5-6-membered aryl ring, or 8-10-membered
     bicyclic aryl ring containing 0-5 heteroatoms, or a 3-7-membered saturated or
     partially unsatd. ring containing 0-3 heteroatoms; R4 = Q-Rx; Q = a bond,
     alkylidene chain wherein up to two non-adjacent methylene units of Q are
     optionally replaced by CO, CO2, COCO, CONH and derivs., SO, SO2, O, S, NH
     and derivs., etc. with proviso; and their pharmaceutically acceptable
     salts], useful as inhibitors of voltage-gated sodium channels and calcium
     channels, were prepared Thus, Pd-cross coupling of 5-ethoxycarbonyl-2-
     chloro-4-(N,N-dimethylamino)pyrimidine (preparation given) with phenylboronic
     acid gave II in 92% yield. Representative compds. I were found to possess
     desired N-type calcium channel modulation activity and selectivity (no
     specific data given). Also, representative compds. I were found to
     possess desired voltage gated sodium channel activity and selectivity (no
     specific data given). The invention also provides pharmaceutically
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acceptable compns. comprising the compds. I and methods of using the compns. in the treatment of various disorders.

IT 823792-42-3P 823792-55-8P 823792-99-0P

823794-38-3P 823794-57-6P 823794-78-1P

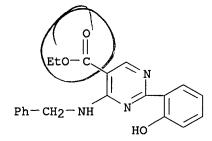
823794-84-9P 823795-27-3P 823796-16-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of pyrimidines as modulators of voltage-gated ion channels)

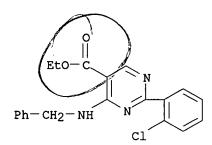
RN 823792-42-3 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 2-(2-hydroxyphenyl)-4-[(phenylmethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)



RN 823792-55-8 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 2-(2-chlorophenyl)-4-[(phenylmethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)



RN 823792-99-0 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 2-phenyl-4-[(phenylmethyl)amino]-6-(4-pyridinyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 823794-38-3 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 2-(2-methoxyphenyl)-4-[(phenylmethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 823794-57-6 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-methyl-2-phenyl-6-[(phenylmethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ \text{Eto-C} & & & \\ & & & \\ \text{Ph-CH}_2-\text{NH} & & & \\ \end{array}$$

RN 823794-78-1 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 2-(2-methylphenyl)-4-[(phenylmethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 823794-84-9 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[methyl(phenylmethyl)amino]-2-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 823795-27-3 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 2,4-diphenyl-6-[(phenylmethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 823796-16-3 CAPLUS

CN 4-Pyrimidinamine, 5-chloro-2-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

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L10
    ANSWER 31 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
     2004:1059317 CAPLUS
ΑN
DN
     142:23305
     Preparation of trisubstituted heteroaromatic compounds as calcium sensing
ΤI
     receptor modulators
IN
     Yang, Wu; Dickson, John K.; Cooper, Christopher B.; Dodd, Dharmpal S.;
     Ruan, Zheming; Schnur, Dora M.
PA
     Bristol-Myers Squibb Company, USA
SO
     PCT Int. Appl., 83 pp.
     CODEN: PIXXD2
DТ
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                        KIND
                               DATE
                                           APPLICATION NO.
                                                                   DATE
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                                           -----
                                                                   _____
PΙ
     WO 2004106296
                         A2
                               20041209
                                           WO 2004-US16713
                                                                   20040527
    WO 2004106296
                         А3
                               20051222
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
            CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
            GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
            LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
            NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
            TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
            AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
            EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
            SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
            SN, TD, TG
     US 2005004151
                               20050106
                                           US 2004-854484
                         A1
                                                                   20040526
PRAI US 2003-473904P
                               20030528
                         Ρ
    MARPAT 142:23305
AB
     Title compds. I [X = C, N; A, B = CH, N and A and B cannot both be CH; R1
     = ArL; R2 = H, alkyl or R1 and R2 can be joined to form a cycloheteroalkyl
     ring; Ar = (hetero)aryl; L = linking group; R3, R4, R6 = H, alkyl,
     cycloalkyl, etc.; R4 = alkyl, cycloalkyl, alkenyl, alkynyl, etc.; R7 =
     alkyl, cycloalkyl, etc.; R8 = H, alkyl or R7 and R8 can be joined together
     to form a 4-7 membered cycloheteroalkyl ring] are prepared For instance, II
     is prepared in 5 steps from pyrazole-1-carboxyimidine and benzylmethylamine.
     I are calcium-sensing receptor modulators; they are useful for the
     treatment of diseases associated with abnormal bone or mineral homeostasis.
IT
     802915-58-8P 802915-59-9P 802915-60-2P
     802915-61-3P 802915-62-4P 802915-68-0P
     802915-69-1P 802915-72-6P 802915-73-7P
     802915-74-8P 802915-79-3P 802915-84-0P
     802915-86-2P 802915-88-4P 802915-91-9P
     802915-95-3P 802915-99-7P 802916-03-6P
     802916-06-9P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of trisubstituted heteroarom. compds. as calcium sensing
        receptor modulators)
RN
     802915-58-8 CAPLUS
CN
     5-Pyrimidinecarboxamide, 2-[methyl(phenylmethyl)amino]-N-(2-phenoxyethyl)-
     4-[4-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)
```

RN 802915-59-9 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[(3-chlorophenyl)methyl]amino]-N-(2-phenoxyethyl)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

RN 802915-60-2 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[(3-chlorophenyl)methyl]amino]-4-(2-chloro-3,4,5-trimethoxyphenyl)-N-(2-phenoxyethyl)- (9CI) (CA INDEX NAME)

RN 802915-61-3 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[ethyl(phenylmethyl)amino]-N-(2-phenoxyethyl)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

RN 802915-62-4 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[(1,3-benzodioxol-5-ylmethyl)amino]-N-(2-phenoxyethyl)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

RN 802915-68-0 CAPLUS

CN 5-Pyrimidinecarboxamide, N-(2-phenoxyethyl)-2-[(2-phenylethyl)amino]-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

RN 802915-69-1 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[(3-methoxyphenyl)methyl]amino]-N-(2-phenoxyethyl)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

RN 802915-72-6 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[2-(4-fluorophenyl)ethyl]amino]-N-(2-phenoxyethyl)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

802915-73-7 CAPLUS RN

5-Pyrimidinecarboxamide, 2-[[(3,5-dichlorophenyl)methyl]amino]-N-(2-CN phenoxyethyl)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

802915-74-8 CAPLUS RN

CN 5-Pyrimidinecarboxamide, N-(2-phenoxyethyl)-2-[(phenylmethyl)amino]-4-(3,4,5-trimethoxyphenyl) - (9CI) (CA INDEX NAME)

RN 802915-79-3 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[(2-hydroxyethyl)(phenylmethyl)amino]-N-(2-phenoxyethyl)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

CN 5-Pyrimidinecarboxamide, 2-[(1,3-benzodioxol-5-ylmethyl)amino]-N-(4-phenylbutyl)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

RN 802915-86-2 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[(1,3-benzodioxol-5-ylmethyl)amino]-N-(3-phenylpropyl)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

RN 802915-88-4 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[[3-(methylthio)phenyl]methyl]amino]-N-(2-phenoxyethyl)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

RN 8.02.9.15=91-9 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[ethyl(phenylmethyl)amino]-N-(4-phenylbutyl)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

RN 802915-95-3 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[(2-chloro-6-methylphenyl)methyl]amino]-N-(2-phenoxyethyl)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

RN 802915-99-7 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[(4-hydroxy-3-methoxyphenyl)methyl]amino]-N-(2-phenoxyethyl)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

RN 802916-03-6 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-[[[4-(dimethylamino)phenyl]methyl]amino]-N-(2-phenoxyethyl)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

802916-06-9 CAPLUS RN

5-Pyrimidinecarboxamide, N-(2-phenoxyethyl)-2-[[[3-(trifluoromethoxy)phenyl]methyl]amino]-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME) CN

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L10
    ANSWER 32 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
     2004:802711 CAPLUS
AN
     141:314020
DN
     Preparation of substituted p-diaminobenzene derivatives as openers of the
TI
     KCNQ family potassium ion channels
IN
     Khanzhin, Nikolay; Rottlaender, Mario; Ritzen, Andreas; Watson, William
     Patrick
PA
     H. Lundbeck A/S, Den.
     PCT Int. Appl., 176 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                            APPLICATION NO.
                                                                   DATE
                                DATE
                         ____
                                _____
                                            ______
ΡI
    WO 2004082677
                                            WO 2004-DK186
                         A1
                                20040930
                                                                   20040318
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
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            GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
        SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
            TD, TG
    AU 2004222626
                          A1
                                20040930
                                            AU 2004-222626
                                                                   20040318
     CA 2519582
                                20040930
                          AΑ
                                            CA 2004-2519582
                                                                   20040318
    EP 1613303
                          A1
                                20060111
                                            EP 2004-721472
                                                                   20040318
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK
    BR 2004008437
                         Α
                                20060404
                                            BR 2004-8437
                                                                   20040318
    CN 1761464
                         Α
                                20060419
                                            CN 2004-80007507
                                                                   20040318
    NO 2005004848
                                            NO 2005-4848
                         Α
                                20051020
                                                                   20051020
PRAI DK 2003-441
                         Α
                                20030321
    US 2003-456698P
                         Р
                                20030321
    WO 2004-DK186
                         W
                                20040318
OS
    MARPAT 141:314020
AB
    The title anilines I \{s = 0-1; U = 0, S, S02, etc.; q = 0-1; X = C0, S02;
    with the proviso that q = 0 when X = SO2; Z = O, S; R1 = H, alk(en/yn)yl,
    cycloalk(en)yl, etc.; R2 = H, alk(en/yn)yl, cycloalk(en)yl, etc.; R3 =
    alk(en/yn)yl, cycloalk(en)yl, heterocycloalk(en)yl, etc.; Y =
     (un) substituted Ph, naphthyl, thienyl, etc.], useful for the prevention,
     treatment or inhibition of a disorder being responsive to an increased ion
     flow in a potassium channel, were prepared and formulated. Thus, reductive
     amination of Pr (4-amino-2-methylphenyl)carbamate (preparation given) with
    benzofuran-2-carbaldehyde in the presence of NaBH3CN afforded 43% Pr
     {4-[(benzofuran-2-ylmethyl)amino]-2-methylphenyl}carbamate. The compds. I
    have an EC50 of <20000nM, in most cases <2000nM and in many cases <200nM
    in KCNQ2 channel assay.
IT
     766518-59-6P 766518-60-9P
    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (preparation of substituted p-diaminobenzene derivs. as openers of the KCNQ
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Page 407

family potassium ion channels)

766518-59-6 CAPLUS

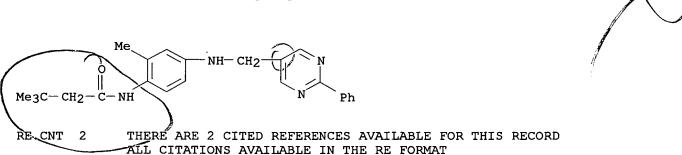
RN

CN Benzeneacetamide, 4-fluoro-N-[2-methyl-4-[[(4-methyl-2-phenyl-5-pyrimidinyl)methyl]amino]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{NH} \\ \text{CH}_2 \\ \text{NH} \\ \text{CH}_2 \\ \text{NH} \\ \text{NH} \\ \text{C} \\ \text{CH}_2 \\ \text{NH} \\ \text{NH} \\ \text{C} \\ \text{CH}_2 \\ \text{NH} \\ \text{C} \\ \text{CH}_2 \\ \text{NH} \\ \text{C} \\ \text{C} \\ \text{NH} \\ \text{C} \\ \text{C}$$

RN 766518-60-9 CAPLUS

CN Butanamide, 3,3-dimethyl-N-[2-methyl-4-[[(2-phenyl-5-pyrimidinyl)methyl]amino]phenyl]- (9CI) (CA INDEX NAME)



10/671,070

L10 ANSWER 33 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:734313 CAPLUS

DN 141:366072

TI Preparation of new N6,9-disubstituted 2-phenyl-adenines and corresponding 8-azaadenines. A feasibility study for application to solid-phase synthesis. I [1]

AU Biagi, Giuliana; Giorgi, Irene; Livi, Oreste; Pacchini, Federica; Scartoni, Valerio; Salerni, Oreste LeRoy.

CS Dipartimento di Scienze Farmaceutiche, Universita di Pisa, Pisa, 56126, Italy

SO Journal of Heterocyclic Chemistry (2004), 41(4), 575-580 CODEN: JHTCAD; ISSN: 0022-152X

PB HeteroCorporation

DT Journal

LA English

OS CASREACT 141:366072

AB A suitably substituted pyrimidine I was converted to a number of title compds. Nucleophilic substitution involving of chlorine by treatment with phenylmethanethiol yielded II or III, depending on the reaction temperature Treatment of III with an amine afforded 6-phenylmethanesulfanyl-N4substituted-2-phenyl-pyrimidine-4,5-diamines. These pyrimidines were converted into 2-phenylpurines and 2-phenyl-8-azapurines, by treatment with tri-Et orthoformate in the presence of hydrochloric acid (or acetic anhydride), or with potassium nitrite and acetic acid resp. The thioether function on C(6) was then converted into a sulfonyl group by oxidation with m-chloroperoxybenzoic acid affording purines and their 8-azaanalogs; these compds., as crude products, were treated with an amine to yield the corresponding adenines or 8-azaadenines. All reactions were performed under conditions compatible with the possible use of a thiomethyl resin in place of phenylmethanethiol to bind the pyrimidine ring of I to a solid phase.

IT 778594-76-6P 778594-77-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of new N6,9-disubstituted 2-phenyl-adenines and corresponding 8-azaadenines from a pyrimidine via nucleophilic substitution for evaluation of feasibility of their solid-phase synthesis)

RN 778594-76-6 CAPLUS

CN 4,5-Pyrimidinediamine, 2-phenyl-N4-(phenylmethyl)-6-[(phenylmethyl)thio]-(9CI) (CA INDEX NAME)

RN 778594-77-7 CAPLUS

CN 4,5-Pyrimidinediamine, N4-[(4-methoxyphenyl)methyl]-2-phenyl-6-[(phenylmethyl)thio]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} & \\ & \text{N} & \\ & \text{N} & \\ & \text{NH} - \text{CH}_2 \end{array} \\ \begin{array}{c} \text{OMe} \\ & \text{NH}_2 \end{array}$$

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 34 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
     2004:718520 CAPLUS
AN
DN
     141:243558
ΤI
     Preparation of pyrimidine derivatives as antiinflammatory agents
     Ohshima, Etsuo; Miyama, Motoki; Yanagawa, Koji; Aratake, Seiji; Miki,
IN
     Ichiro; Kobayashi, Katsuya; Sato, Takashi; Kawabe, Ari; Iwase, Miho
     Kyowa Hakko Kogyo Co., Ltd., Japan
PA
     PCT Int. Appl., 87 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     Japanese
FAN.CNT 1
     PATENT NO.
                           KIND
                                   DATE
                                                APPLICATION NO.
                                                                          DATE
                                   20040902
PΙ
     WO 2004074260
                            A1
                                                WO 2004-JP1962
                                                                          20040220
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             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE,
             BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                            A1 / 20051116 | EP 2004-713192
     EP 1595869
                                                                          20040220
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
PRAI JP 2003-44174
                            Α
                                   20030221
     JP 2003-314058
                            Α
                                   20030905
     WO 2004-JP1962
                            W
                                   20040220
OS
     MARPAT 141:243558
AB
     The title pyrimidine derivs with general formula of I [wherein Ar =
     (un) substituted aryl or heteroaryl; R1 = (un) substituted amino; A = a
     single bond, (un) substituted piperidinyl, or piperazinyl; Q =
     (un) substituted amino, piperidin-4-ylamino, etc.] or quaternary ammonium
     salts or pharmaceutically acceptable salts thereof are prepared For
     example, the compound II was prepared in a multi-step synthesis in good yield.
     II inhibited 91% binding of thymus and activation-regulated chemokine
     (TARC) towards Hut78 cell in cow. I have an antiinflammatory effect and a
     TARC and/or MDC function-controlling effect and are useful in treating
     and/or preventing various diseases in which T cells participate, for
     example, allergic diseases, autoimmune diseases, rejection at
     transplantation, etc. (no data). Formulations containing I as an active
     ingredient were also described.
IT
     749859-72-1P 749859-73-2P 749859-74-3P
     749860-06-8P
     RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
     preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (drug candidate; preparation of pyrimidine derivs. as antiinflammatory
        agents)
RN
     749859-72-1 CAPLUS
CN
     4-Pyrimidinamine, 5-(2,4-difluorophenyl)-N-[(2,4-difluorophenyl)methyl]-2-
     (3-methyl[1,4'-bipiperidin]-1'-yl)- (9CI) (CA INDEX NAME)
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RN 749859-73-2 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-5-(2,4-difluorophenyl)-N-[(2,4-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)

RN 749859-74-3 CAPLUS

CN 4-Pyrimidinamine, 5-(2,4-difluorophenyl)-N-[(2,4-difluorophenyl)methyl]-2-(2-methyl[1,4'-bipiperidin]-1'-yl)- (9CI) (CA INDEX NAME)

RN 749860-06-8 CAPLUS
CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[(2,6difluorophenyl)methyl]-5-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)

IT 749859-75-4P 749859-76-5P 749859-77-6P 749859-78-7P 749859-79-8P 749859-80-1P 749859-81-2P 749859-82-3P 749859-83-4P 749859-84-5P 749859-85-6P 749859-86-7P 749859-87-8P 749859-88-9P 749859-89-0P 749859-90-3P 749859-91-4P 749859-92-5P 749859-93-6P 749859-97-0P 749859-98-1P 749859-99-2P 749860-00-2P 749860-01-3P 749860-02-4P 749860-03-5P 749860-04-6P 749860-05-7P 749860-07-9P 749860-08-0P 749860-11-5P 749860-12-6P 749860-13-7P 749860-14-8P 749860-16-0P 749860-17-1P 749860-18-2P 749860-22-8P 749860-23-9P 749860-29-5P 749860-30-8P 749860-31-9P 749860-32-0P 749860-33-1P 749860-34-2P 749860-35-3P 749860-36-4P 749860-41-1P 749860-42-2P 749860-43-3P 749860-44-4P 749860-45-5P 749860-46-6P 749860-47-7P 749860-48-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of pyrimidine derivs. as antiinflammatory agents)

RN 749859-75-4 CAPLUS

CN 4-Pyrimidinamine, 5-(2,4-difluorophenyl)-N-[(2,4-difluorophenyl)methyl]-2-(4-methyl[1,4'-bipiperidin]-1'-yl)- (9CI) (CA INDEX NAME)

RN 749859-76-5 CAPLUS

CN 4-Pyrimidinamine, 5-(2,4-difluorophenyl)-N-[(2,4-difluorophenyl)methyl]-2[(3R,5S)-3,5-dimethyl[1,4'-bipiperidin]-1'-yl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 749859-77-6 CAPLUS

CN 4-Pyrimidinamine, 5-(2,4-difluorophenyl)-N-[(2,4-difluorophenyl)methyl]-2-(3-ethyl[1,4'-bipiperidin]-1'-yl)- (9CI) (CA INDEX NAME)

RN 749859-78-7 CAPLUS

CN [1,4'-Bipiperidine]-3-methanol, 1'-[5-(2,4-difluorophenyl)-4-[[(2,4-difluorophenyl)methyl]amino]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 749859-79-8 CAPLUS

CN [1,4'-Bipiperidine]-3-carboxamide, 1'-[5-(2,4-difluorophenyl)-4-[[(2,4-difluorophenyl)methyl]amino]-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 749859-80-1 CAPLUS

CN [1,4'-Bipiperidine]-3-carboxylic acid, 1'-[5-(2,4-difluorophenyl)-4-[[(2,4-difluorophenyl)methyl]amino]-2-pyrimidinyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 749859-81-2 CAPLUS

CN 4-Pyrimidinamine, 2-[4-(butylmethylamino)-1-piperidinyl]-5-(2,4-difluorophenyl)-N-[(2,4-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)

RN 749859-82-3 CAPLUS

CN 4-Pyrimidinamine, N-[(2,4-difluorophenyl)methyl]-5-(2-fluorophenyl)-2-(3-methyl[1,4'-bipiperidin]-1'-yl)- (9CI) (CA INDEX NAME)

RN 749859-83-4 CAPLUS

CN 4-Pyrimidinamine, N-[(2,4-difluorophenyl)methyl]-2-[(3R,5S)-3,5-dimethyl[1,4'-bipiperidin]-1'-yl]-5-(2-fluorophenyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 749859-84-5 CAPLUS

CN 4-Pyrimidinamine, N-[(2,4-dichlorophenyl)methyl]-5-(2,4-difluorophenyl)-2-(3-methyl[1,4'-bipiperidin]-1'-yl)- (9CI) (CA INDEX NAME)

RN 749859-85-6 CAPLUS

CN 4-Pyrimidinamine, N-[(2,4-dichlorophenyl)methyl]-5-(2,4-difluorophenyl)-2-[4-[2-(1-piperidinyl)ethyl]-1-piperazinyl]- (9CI) (CA INDEX NAME)

$$C1$$
 CH_2
 NH
 N
 N
 N
 CH_2
 CH_2

RN 749859-86-7 CAPLUS

CN 4-Pyrimidinamine, 5-(2,4-difluorophenyl)-N-[(2,6-difluorophenyl)methyl]-2-(3-methyl[1,4'-bipiperidin]-1'-yl)- (9CI) (CA INDEX NAME)

RN 749859-87-8 CAPLUS

CN 4-Pyrimidinamine, 5-(2,4-difluorophenyl)-N-[(2,6-difluorophenyl)methyl]-2[(3R,5S)-3,5-dimethyl[1,4'-bipiperidin]-1'-yl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 749859-88-9 CAPLUS

CN 4-Pyrimidinamine, N-[(2,6-difluorophenyl)methyl]-2-[(3R,5S)-3,5-dimethyl[1,4'-bipiperidin]-1'-yl]-5-(2-fluorophenyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 749859-89-0 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[(2,6-difluorophenyl)methyl]-5-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 749859-90-3 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[(2,6-difluorophenyl)methyl]-5-(1-naphthalenyl)- (9CI) (CA INDEX NAME)

RN 749859-91-4 CAPLUS

CN 4-Pyrimidinamine, 5-[1,1'-biphenyl]-2-yl-2-[1,4'-bipiperidin]-1'-yl-N[(2,6-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)

RN 749859-92-5 CAPLUS

CN 4-Pyrimidinamine, 5-[1,1'-biphenyl]-3-yl-2-[1,4'-bipiperidin]-1'-yl-N[(2,6-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)

RN 749859-93-6 CAPLUS

CN 4-Pyrimidinamine, 5-[1,1'-biphenyl]-4-yl-2-[1,4'-bipiperidin]-1'-yl-N-[(2,6-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)

RN 749859-97-0 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[(2,6-difluorophenyl)methyl]-5-(2-methylphenyl)- (9CI) (CA INDEX NAME)

RN 749859-98-1 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[(2,6-difluorophenyl)methyl]-5-(3-methylphenyl)- (9CI) (CA INDEX NAME)

RN 749859-99-2 CAPLUS
CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[(2,6-difluorophenyl)methyl]-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)

RN 749860-00-2 CAPLUS
CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[(2,6-difluorophenyl)methyl]-5-(2-fluorophenyl)- (9CI) (CA INDEX NAME)

RN 749860-01-3 CAPLUS CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[(2,6difluorophenyl)methyl]-5-(3-fluorophenyl)- (9CI) (CA INDEX NAME)

RN 749860-02-4 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[(2,6-difluorophenyl)methyl]-5-(4-fluorophenyl)- (9CI) (CA INDEX NAME)

RN 749860-03-5 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-5-(2-chlorophenyl)-N-[(2,6-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)

RN 749860-04-6 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-5-(3-chlorophenyl)-N-[(2,6-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)

RN 749860-05-7 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-5-(4-chlorophenyl)-N-[(2,6-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)

RN 749860-07-9 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[(2,6-difluorophenyl)methyl]-5-(3-methoxyphenyl)- (9CI) (CA INDEX NAME)

RN 749860-08-0 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[(2,6-difluorophenyl)methyl]-5-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

RN 749860-11-5 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-5-(2,4-difluorophenyl)-N[(2,6-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)

RN 749860-12-6 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-5-(2,5-difluorophenyl)-N[(2,6-difluorophenyl)methyl]- (9CI) (CA INDEX NAME)

RN 749860-13-7 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[(2,6-difluorophenyl)methyl]-5-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX

NAME)

RN 749860-14-8 CAPLUS

CN Benzonitrile, 3-[2-[1,4'-bipiperidin]-1'-yl-4-[[(2,6-difluorophenyl)methyl]amino]-5-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 749860-16-0 CAPLUS

CN Phenol, 2-[2-[1,4'-bipiperidin]-1'-yl-4-[[(2,6-difluorophenyl)methyl]amino]-5-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 749860-17-1 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[(2,6-difluorophenyl)methyl]-5-(2-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 749860-18-2 CAPLUS
CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[(2,6-difluorophenyl)methyl]-5-phenyl- (9CI) (CA INDEX NAME)

RN 749860-22-8 CAPLUS
CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[(2,4-difluorophenyl)methyl]-5-(2-fluorophenyl)- (9CI) (CA INDEX NAME)

RN 749860-23-9 CAPLUS
CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[(2,6-dichlorophenyl)methyl]-5-(2-fluorophenyl)- (9CI) (CA INDEX NAME)

RN 749860-29-5 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[(4-chloro-2-fluorophenyl)methyl]-5-(2,4-difluorophenyl)- (9CI) (CA INDEX NAME)

RN 749860-30-8 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-5-(2,4-difluorophenyl)-N-[(2-nitrophenyl)methyl]- (9CI) (CA INDEX NAME)

RN 749860-31-9 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-5-(2,4-difluorophenyl)-N-[(4-fluorophenyl)methyl]- (9CI) (CA INDEX NAME)

RN 749860-32-0 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[(2-chloro-6-fluorophenyl)methyl]-5-(2,4-difluorophenyl)- (9CI) (CA INDEX NAME)

RN 749860-33-1 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[2-(4-chlorophenyl)ethyl]-5-(2,4-difluorophenyl)- (9CI) (CA INDEX NAME)

RN 749860-34-2 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[2-(2-chlorophenyl)ethyl]-5-(2,4-difluorophenyl)- (9CI) (CA INDEX NAME)

RN 749860-35-3 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[2-(2,4-dichlorophenyl)ethyl]-5-(2,4-difluorophenyl)- (9CI) (CA INDEX NAME)

RN 749860-36-4 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-5-(2,4-difluorophenyl)-N-[2-(4-fluorophenyl)ethyl]- (9CI) (CA INDEX NAME)

RN 749860-41-1 CAPLUS

CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-5-(2,4-difluorophenyl)-N-[[4-(methylsulfonyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 749860-42-2 CAPLUS
CN 4-Pyrimidinamine, 2-[1,4'-bipiperidin]-1'-yl-N-[2-(2,6-dichlorophenyl)ethyl]-5-(2,4-difluorophenyl)- (9CI) (CA INDEX NAME)

RN 749860-43-3 CAPLUS
CN 1,4'-Bipiperidinium, 1'-[5-(2,4-difluorophenyl)-4-[[(2,4-difluorophenyl)methyl]amino]-2-pyrimidinyl]-1-methyl-, iodide (9CI) (CA INDEX NAME)

• I-

RN 749860-44-4 CAPLUS
CN 1,4'-Bipiperidinium, 1'-[5-(2,4-difluorophenyl)-4-[[(2,4-difluorophenyl)methyl]amino]-2-pyrimidinyl]-1-ethyl-, iodide (9CI) (CA INDEX NAME)

• I-

RN 749860-45-5 CAPLUS
CN 1,4'-Bipiperidinium, 1'-[5-(2,4-difluorophenyl)-4-[[(2,4-difluorophenyl)methyl]amino]-2-pyrimidinyl]-1-propyl-, iodide (9CI) (CA INDEX NAME)

• I-

• Br-

RN 749860-47-7 CAPLUS
CN 1,4'-Bipiperidinium, 1'-[5-(2,4-difluorophenyl)-4-[[(2,4-difluorophenyl)methyl]amino]-2-pyrimidinyl]-1,2-dimethyl-, iodide (9CI) (CA INDEX NAME)

• I-

RN 749860-48-8 CAPLUS
CN 1,4'-Bipiperidinium, 1'-[5-(2,4-difluorophenyl)-4-[[(2,4-difluorophenyl)methyl]amino]-2-pyrimidinyl]-1,3-dimethyl-, iodide (9CI) (CA INDEX NAME)

• I-

$$\begin{array}{c|c}
C1 \\
N \\
N \\
NH-CH_2 \\
F
\end{array}$$

RN 749860-51-3 CAPLUS

CN 4-Pyrimidinamine, 2-chloro-N-[(2,4-difluorophenyl)methyl]-5-(2-fluorophenyl)- (9CI) (CA INDEX NAME)

RN 749860-52-4 CAPLUS

CN 4-Pyrimidinamine, 2-chloro-N-[(2,4-dichlorophenyl)methyl]-5-(2,4-difluorophenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} C1 & & C1 \\ N & N & \\ N & NH-CH_2 & \\ \hline F & & C1 \\ \end{array}$$

RN 749860-57-9 CAPLUS

CN 4-Pyrimidinamine, 2-chloro-N-[(2,6-difluorophenyl)methyl]-5-(2-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 749860-60-4 CAPLUS

CN 4-Pyrimidinamine, 2-chloro-N-[(2,6-difluorophenyl)methyl]-5-phenyl- (9CI) (CA INDEX NAME)

RN 749860-66-0 CAPLUS

CN 4-Pyrimidinamine, N-[(2,4-difluorophenyl)methyl]-5-(2-fluorophenyl)-2-(methylthio)- (9CI) (CA INDEX NAME)

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 35 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:626175 CAPLUS

DN 141:260694

- TI Substituted benzylamino-6-(trifluoromethyl)pyrimidin-4(1H)-ones: a novel class of selective human A-FABP inhibitors
- AU Ringom, Rune; Axen, Eva; Uppenberg, Jonas; Lundbaeck, Thomas; Rondahl, Lena; Barf, Tjeerd
- CS Department of Medicinal Chemistry, Biovitrum AB, Uppsala, SE-751 37, Swed.
- SO Bioorganic & Medicinal Chemistry Letters (2004), 14(17), 4449-4452 CODEN: BMCLE8; ISSN: 0960-894X
- PB Elsevier B.V.
- DT Journal
- LA English
- OS CASREACT 141:260694
- AB The synthesis and evaluation of human A-FABP inhibitors based on 6-(trifluoromethyl)pyrimidine-4(1H)-ones, e.g., I, is described. Two series of compds., bearing either an amino or carbon substituent in the 2-position of the pyrimidine ring were investigated. Modification of substituents and chain length optimization led to compds. with low micromolar activity and good selectivity for human A-FABP.
- IT 756525-63-0P 756525-64-1P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation, human A-FABP binding affinity, and structure-activity relationship of (benzylamino)pyrimidinones via condensation of chlorobenzylamine with methylisothiourea sulfate followed by heterocyclization with acetoacetates)

RN 756525-63-0 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[[(4-chlorophenyl)methyl]amino]-6-phenyl- (9CI) (CA INDEX NAME)

RN 756525-64-1 CAPLUS

CN 4(1H)-Pyrimidinone, 2-[[(4-chlorophenyl)methyl]amino]-6-(2-fluorophenyl)-(9CI) (CA INDEX NAME)

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L10
     ANSWER 36 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2004:589250 CAPLUS
DN
     141:140470
ΤI
     Preparation of aminophenylbenzamides as inhibitors of histone deacetylase
IN
     Delorme, Daniel; Zhou, Zhihong
PA
     Methylgene, Inc., Can.
SO
     U.S. Pat. Appl. Publ., 318 pp., Cont.-in-part of U.S. Ser. No. 242,304.
     CODEN: USXXCO
DT
     Patent
LА
     English
FAN.CNT 3
     PATENT NO.
                           KIND
                                   DATE
                                                 APPLICATION NO.
                                                                           DATE
                                   _____
PΙ
     US 2004142953
                           A1
                                   20040722
                                                US 2003-358556
                                                                           20030204
     US 6897220
                                   20050524
                            B2
     US 2004106599
                                                 US 2002-242304
                            A1
                                   20040603
                                                                           20020912
     AU 2004210016
                            A1
                                   20040819
                                                 AU 2004-210016
                                                                           20040204
     CA 2515338
                                                 CA 2004-2515338
                            AΑ
                                   20040819
                                                                           20040204
     WO 2004069823
                            A1
                                   20040819
                                                 WO 2004-CA139
                                                                           20040204
          W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
              CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
              GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
         CL, GH, GH, HR, HO, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     EP 1590340
                            A1
                                   20051102
                                                 EP 2004-707852
                                                                           20040204
              AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
                                                CN 2004-80001769
     CN 1723207
                            Α
                                   20060118
                                                                          20040204
     BR 2004007195
                            Α
                                   20060214
                                                 BR 2004-7195
                                                                           20040204
     JP 2006514998
                            T2
                                   20060518
                                                 JP 2005-518241
                                                                           20040204
     US 2006058298
                            A1
                                   20060316
                                                 US 2005-81095
                                                                           20050315
     JP 2005255683
                            A2
                                   20050922
                                                 JP 2005-80310
                                                                          20050318
     US 2005288282
                            A1
                                                 US 2005-91025
                                   20051229
                                                                           20050325
PRAI US 2001-322402P
                           P
                                   20010914
     US 2002-391728P
                           P
                                   20020626
                            A2
     US 2002-242304
                                   20020912
     JP 2003-528544
                            A3
                                   20020912
     US 2003-358556
                                   20030204
                            Α
     WO 2004-CA139
                            W
                                   20040204
     MARPAT 141:140470
os
AB
     Title compds. e.g. (I; Y, Z = N, CH; W = Q1, Q2, Q3, etc.), were prepared
     Thus, 4-[(4-Amino-6-(2-indanylamino)-[1,3,5]triazin-2-
     yl)amino]methyl]benzoic acid (preparation given) in DMF was stirred with Et3N,
     BOP, and 1,2-phenylenediamine to give 63% 4-[[(4-Amino-6-(2-indanylamino)-
     [1,3,5]triazin-2-yl)amino]methyl]-N-(2-aminophenyl)benzamide. The latter
     inhibited human histone deacetylase HDAC-1 with IC50 = 0.4 \muM.
IT
     503043-79-6P, N-(2-Aminophenyl)-4-(((4-chloro-6-(3,4-
     dimethoxyphenyl)pyrimidin-2-yl)amino)methyl)benzamide 503043-80-9P
     , N-(2-Aminophenyl)-4-(((4-(3,4-dimethoxyphenyl)pyrimidin-2-
     yl)amino)methyl)benzamide
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
         (drug candidate; preparation of aminophenylbenzamides as inhibitors of
```

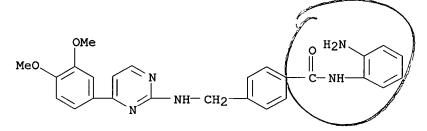
histone deacetylase for treating cell proliferative disorders)

RN 503043-79-6 CAPLUS

CN Benzamide, N-(2-aminophenyl)-4-[[[4-chloro-6-(3,4-dimethoxyphenyl)-2-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)

RN 503043-80-9 CAPLUS

CN Benzamide, N-(2-aminophenyl)-4-[[[4-(3,4-dimethoxyphenyl)-2-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)



RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 37 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
L10
AN
     2004:589247 CAPLUS
DN
     141:140463
     Preparation of heterocyclic compounds as selective phosphodiesterase V
TI
     inhibitors
IN
     Yamada, Koichiro; Matsuki, Kenji; Omori, Kenji; Kikkawa, Kohei
PA
     U.S. Pat. Appl. Publ., 116 pp., Cont.-in-part of U.S. Ser. No. 258,545.
so
     CODEN: USXXCO
DT
     Patent
     English
LА
FAN.CNT 3
                                 DATE
     PATENT NO.
                         KIND
                                             APPLICATION NO.
                                                                      DATE
                          ----
                                 -----
                                             _____
                                             US 2003-699804
PΙ
     US 2004142930
                          A1
                                 20040722
                                                                      20031104
     JP 2002012587
                                             JP 2000-277652
                          A2
                                 20020115
                                                                      20000913
     JP 3637961
                          В2
                                 20050413
                          A1
     WO 2001083460
                                             WO 2001-JP2034
                                                                      20010315
                                 20011108
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM,
             HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT,
             LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
             SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
             YU, ZA, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     US 2003229089
                          Α1
                                 20031211
                                             US 2002-258545
PRAI JP 2000-130371
                                 20000428
                          Α
     JP 2000-277652
                                 20000913
                          Α
     WO 2001-JP2034
                                 20010315
                          W
     US 2002-258545
                                 20021025
                          A2
     JP 1999-261852
                          Α
                                 19990916
OS
     MARPAT 141:140463
AB
     The title compds. (I) [X = CH, N; Y = NH, NR, S, O, CH:N, N:CH, N:N,
     CH:CHC(:R5)N, CH:C(R5), N:C(R7); R1 = each (un)substituted lower alkoxy,
     amino, heterocyclyl containing N atom(s), HO, or heterocyclyloxy containing N
     atom(s), cyano; R2 = lower alkylamino or lower alkoxy each optionally
     substituted by an (un)substituted aryl, lower alkoxy group substituted by
     an aromatic heterocyclic ring containing N atom(s), lower alkylamino group
     substituted by a (un)substituted heterocyclic ring, (un)substituted
     arylamino; R3 = each (un)substituted aryl, heterocyclyl containing N atom(s),
     lower alkyl, lower alkoxy, lower cycloalkoxy, heterocyclyloxy containing N
     atom(s), or NH2; R4-R7 = each (un) substituted aryl, heterocyclyl containing N
     atom(s), lower alkoxy, or NH2; R4, R5, R6 or R7 may combine with R3 to
     form a lactone ring Q or Q1; when X = N, Y = CH:N, or N:CH, R2 = an amino
     group monosubstituted by an (un) substituted arylmethyl, and R3 =
     (un) substituted lower alkyl, amino monosubstituted by an (un) substituted
     heterocyclyl-lower alkyl containing N atom(s) in the ring, heterocyclylamino
     containing N atom(s) in the ring, or (un) substituted lower cycloalkylamino, R1
     = each (un)substituted lower alkoxy, amino, heterocyclyloxy containing N
     atom(s) in the ring, or cyano group] or pharmacol. acceptable salts
     thereof are prepared These compds. have excellent selective PDE V
     inhibitory activity and therefore, are useful as therapeutic or
     prophylactic drugs for treating various diseases due to functional
     disorders on cGMP-signaling, such as erectile dysfunction, pulmonary
     hypertension, and diabetic gastroparesis. Thus, 2-(hydroxymethyl)pyridine
     was treated with NaH in THF and etherified with 2-chloro-5-(3,4,5-
```

trimethoxyphenylcarbonyl) -4-(3-chloro-4-methoxybenzylamino)pyrimidine to give 2-(2-pyridylmethoxy) -5-(3,4,5-trimethoxyphenylcarbonyl) -4-(3-chloro-4-methoxybenzylamino)pyrimidine.

IT 372117-36-7P 372117-37-8P 372117-38-9P 372117-39-0P 372117-40-3P 372117-41-4P 372117-44-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heterocyclic compds. as selective phosphodiesterase V inhibitors for treating various diseases due to functional disorders on cGMP-signaling)

RN 372117-36-7 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[(3-chloro-4-methoxyphenyl)methyl]amino]-2-(2-pyridinylmethoxy)-6-(3,4,5-trimethoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 372117-37-8 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[(3-chloro-4-methoxyphenyl)methyl]amino]-2-(4-hydroxy-1-piperidinyl)-6-(3,4,5-trimethoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)

Page 444

RN 372117-38-9 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[(3-chloro-4-methoxyphenyl)methyl]amino]-2[2-(hydroxymethyl)-4-morpholinyl]-6-(3,4,5-trimethoxyphenyl)-, methyl
ester (9CI) (CA INDEX NAME)

CN 5-Pyrimidinecarboxylic acid, 4-[[(3-chloro-4-methoxyphenyl)methyl]amino]-2[(2-methoxyethyl)methylamino]-6-(3,4,5-trimethoxyphenyl)-, methyl ester
(9CI) (CA INDEX NAME)

Me
$$C1 MeO-CH_2-CH_2-N OMe$$
 OMe CH_2-NH OMe OM

CN 5-Pyrimidinecarboxylic acid, 4-[[(3-chloro-4-methoxyphenyl)methyl]amino]-2[2-(dimethylamino)ethoxy]-6-(3,4,5-trimethoxyphenyl)-, methyl ester (9CI)
(CA INDEX NAME)

CN 5-Pyrimidinecarboxylic acid, 4-[[(3-chloro-4-methoxyphenyl)methyl]amino]-2-(1-piperazinyl)-6-(3,4,5-trimethoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 372117-44-7 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 2-[bis(2-hydroxyethyl)amino]-4-[[(3-chloro-4-methoxyphenyl)methyl]amino]-6-(3,4,5-trimethoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{CH}_2-\text{CH}_2-\text{OH} \\ \text{C1} \quad \text{HO-CH}_2-\text{CH}_2-\text{N} \\ \text{OMe} \\ \text{OMe} \\ \text{OMe} \\ \text{O} \\ \end{array}$$

```
L10
     ANSWER 38 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2004:467883 CAPLUS
DN
     141:38627
TI
     Preparation of 2,4,6-trisubstituted pyrimidines as phosphatidylinositol
     (pi) 3-kinase inhibitors and their use in the treatment of cancer
TN
     Nuss, John M.; Pecchi, Sabina; Renhowe, Paul A.
PΑ
     Chiron Corporation, USA
     PCT Int. Appl., 151 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                          KIND
                                 DATE
                                             APPLICATION NO.
                                                                      DATE
                                             WO 2003-US37294
PΙ
     WO 2004048365
                           A1
                                 20040610
                                                                      20031121
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             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO
             NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,
             TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,
             TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD,
                                             CA 2003-2507100
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                                 20040610
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     AU 2003295776
                           A1
                                 20040618
                                             AU 2003-295776
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     US 2004176385
                           A1
                                 20040909
                                             US 2003-719896
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     EP 1575940
                           A1
                                 20050921
                                             EP 2003-786980
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             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     BR 2003016485
                                 20051011
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                                                                      20031121
     CN 1735607
                           Α
                                 20060215
                                             CN 2003-80108239
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     JP 2006514118
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                                             JP 2005-510381
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     NO 2005002927
                           Α
                                 20050708
                                             NO 2005-2927
                                                                      20050615
PRAI US 2002-428473P
                           Р
                                 20021121
     US 2003-438568P
                           Ρ
                                 20030107
     US 2003-523081P
                           Ρ
                                 200311197
     WO 2003-US37294
                           W
                                 20031121
OS
     MARPAT 141:38627
AB
     Title compds. I [Y = (un)substituted alk(en/yn)yl, hetero/aryl,
     heterocyclyl; X = a direct link, NH and derivs., CH2 and derivs., O, S,
     SO, SO2, etc.; R1 = H, alkyl, CO2H, halo, OH and derivs., NH2 and derivs.;
     R2 = (un)substituted hetero/aryl, heterocyclyl; W = NH2 and derivs.,
     (un) substituted alkyl, cyclyl containing at least one heteroatom; with
     provisos; their stereoisomers, tautomers, pharmaceutically acceptable
     salts, esters, or prodrugs] were prepared as phosphatidylinositol (pi)
     3-kinase inhibitors for treating neoplasm. A solid phase synthesis is
     given for pyrimidine II-2CF3CO2H.
                                         Selected I displayed an IC50 < 20
     μM in a cell proliferation assay.
IT
     701243-19-8P, 3-[6-[(4-Methylbenzyl)[(pyridin-2-yl)methyl]amino]-2-
     (morpholin-4-yl)pyrimidin-4-yl]phenol 701243-23-4P,
     3-[6-(Dibenzylamino)-2-(morpholin-4-yl)pyrimidin-4-yl]phenol
     701243-24-5P, 3-[6-[(Benzyl)(1,3-thiazol-2-ylmethyl)amino]-2-
     (morpholin-4-yl)pyrimidin-4-yl]phenol 701243-58-5P,
     3-[6-[(4-Methylbenzyl)[(pyridin-3-yl)methyl]amino]-2-(morpholin-4-
     yl)pyrimidin-4-yl]phenol
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
```

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(phosphatidylinositol 3-kinase inhibitor; preparation of 2,4,6-trisubstituted pyrimidines as phosphatidylinositol 3-kinase inhibitors for treating neoplasm)

RN 701243-19-8 CAPLUS

CN Phenol, 3-[6-[[(4-methylphenyl)methyl](2-pyridinylmethyl)amino]-2-(4-morpholinyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 701243-23-4 CAPLUS

CN Phenol, 3-[6-[bis(phenylmethyl)amino]-2-(4-morpholinyl)-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

RN 701243-24-5 CAPLUS

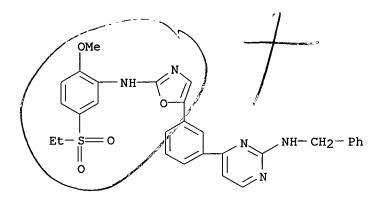
CN Phenol, 3-[2-(4-morpholinyl)-6-[(phenylmethyl)(2-thiazolylmethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN

701243-58-5 CAPLUS
Phenol, 3-[6-[[(4-methylphenyl)methyl](3-pyridinylmethyl)amino]-2-(4-morpholinyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME) CN

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 39 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
ΑN
     2004:331949 CAPLUS
     140:339318
DN
ΤI
     Preparation of 1,3-oxazol-2-amines as VEGFR2, CDK2, and CDK4 inhibitors
IN
     Brown, Matthew Lee; Cheung, Mui; Dickerson, Scott Howard; Gauthier,
     Cassandra; Harris, Philip Anthony; Hunter, Robert Neil, III; Pacofsky,
     Gregory; Peel, Michael Robert; Stafford, Jeffrey Alan
PA
     Smithkline Beecham Corporation, USA
     PCT Int. Appl., 213 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                                                                         DATE
                           KIND
                                  DATE
                                               APPLICATION NO.
                           ----
PΙ
     WO 2004032882
                           A2
                                  20040422
                                               WO 2003-US33317
                                                                         20031010
     WO 2004032882
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                                  20040708
             AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
              CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
              GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
              LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ,
              OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
              TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     AU 2003287178
                            A1
                                  20040504
                                               AU 2003-287178
                                                                         20031010
     EP 1551813
                            A2
                                 - 20050713
                                               EP 2003-781357
                                                                         20031010
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     JP 2006503081
                                               JP 2004-543799
                            Т2
                                  20060126
                                                                         20031010
     US 2005288515
                            A1
                                  20051229
                                               US 2005-530810
                                                                         20050408
PRAI US 2002-417548P
                           Ρ
                                  20021010 ===
     WO 2003-US33317
                            W
                                  20031010
os
     MARPAT 140:339318
AB
     The title compds. [I; D1 = (un) substituted aryl, heteroaryl, heterocyclyl;
     D2 = H, alkyl; D3 = (un)substituted aryl, heteroaryl] which are useful as
     VEGFR2, CDK2, and CDK4 inhibitors in the treatment of hyperproliferative
     diseases, were prepared E.g., a 5-step synthesis of I [D1 = 3-MeOC6H4; D2 =
     H; D3 = Ph], starting from 2-bromo-1-(3-methoxyphenyl)ethanone, was given.
     Different compds. I are particularly effective at inhibiting CDK2 and/or
     CDK4 enzymes at 0.0001 to 1 µM and addnl. show specificity relative to
                      The specific data for representative compds. I are given.
     The pharmaceutical compns. comprising the compound I are claimed.
IT
     681004-26-2P, N-Benzyl-4-[3-(2-[[5-(ethylsulfonyl)-2-
     methoxyphenyl]amino]-1,3-oxazol-5-yl)phenyl]pyrimidin-2-amine
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
         (preparation of 1,3-oxazol-2-amines as VEGFR2, CDK2, and CDK4 inhibitors for
        treating cancer)
RN
     681004-26-2 CAPLUS
     2-Pyrimidinamine, 4-[3-[2-[[5-(ethylsulfonyl)-2-methoxyphenyl]amino]-5-
CN
     oxazolyl]phenyl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)
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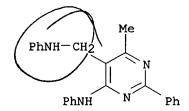


- L10 ANSWER 40 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2004:298615 CAPLUS
- DN 142:74519
- TI Synthesis of pyrimido[4,5-d]pyrimidine derivatives
- AU Cieplik, J.
- CS Department of Organic Chemistry, Medical Academy, Wroclaw, 50-137, Pol.
- SO Annales Universitatis Mariae Curie-Sklodowska, Sectio AA: Chemia (2003), 58, 105-111
 - CODEN: AUMCD7; ISSN: 0137-6853
- PB Wydawnictwo Uniwersytetu Marii Curie-Sklodowskiej
- DT Journal
- LA English
- OS CASREACT 142:74519
- AB The synthesis of pyrimido[4,5-d]pyrimidine derivs. I (R = H, Et, Ph), where identical structures have been obtained by different methods, is presented.
- IT 812665-65-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyrimidopyrimidines via substitution of anilino(chloromethyl)pyrimidines with amines followed by intramol. Mannich reaction with formaldehyde)

- RN 812665-65-9 CAPLUS
- CN 5-Pyrimidinemethanamine, 4-methyl-N,2-diphenyl-6-(phenylamino)- (9CI) (CA INDEX NAME)



RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 41 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
L10
ΑN
     2004:292069 CAPLUS
DN
     140:303694
ΤI
     Preparation of substituted pyrimidines for treating disorders mediated by
     the Cannabinoid-1 receptor
IN
     Kopka, Ihor E.; Li, Bing; Hagmann, William K.
PA
     Merck & Co., Inc., USA
     PCT Int. Appl., 181 pp.
SO
     CODEN: PIXXD2
DΤ
     Patent
     English
LА
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                    DATE
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                                             ______
                                _____
ΡI
     WO 2004029204
                          A2
                                20040408
                                            WO 2003-US30161
                                                                    20030923
     WO 2004029204
                                20040617
                          А3
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
             GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
             TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                20040408
     CA 2499497
                          AΑ
                                            CA 2003-2499497
                                                                    20030923
     AU 2003275242
                                            AU 2003-275242
                                20040419
                          Α1
                                                                    20030923
     EP 1546115
                          A2
                                20050629
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                                                                    20030923
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     JP 2006510597
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                                20060330
                                            JP 2004-539876
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     US 2005245554
                          A1
                                20051103
                                            US 2005-527561
                                                                    20050311
PRAI US 2002-414144P
                          Р
                                20020927 -
     WO 2003-US30161
                          W
                                20030923
OS
     MARPAT 140:303694
AΒ
     Novel pyrimidines (shown as I; variables defined below; e.g. II) are
     antagonists and/or inverse agonists of the Cannabinoid-1 (CB1) receptor
     (no data) and are useful in the treatment, prevention and suppression of
     diseases mediated by the CB1 receptor (no data). The compds. of the
     present invention are useful as centrally acting drugs in the treatment of
     psychosis, memory deficits, cognitive disorders, migraine, neuropathy,
     neuro-inflammatory disorders including multiple sclerosis and
     Guillain-Barre syndrome and the inflammatory sequelae of viral
     encephalitis, cerebral vascular accidents, and head trauma, anxiety
     disorders, stress, epilepsy, Parkinson's disease, movement disorders, and
     schizophrenia. The compds. are also useful for the treatment of substance
     abuse disorders, the treatment of obesity or eating disorders, as well as
     the treatment of asthma, constipation, chronic intestinal
     pseudo-obstruction, and cirrhosis of the liver. Although the methods of
     preparation are not claimed, .apprx.130 example prepns. of I and 17 example
     prepns. of intermediates are included. For example, 2-(4-fluorobenzyloxy)-
     4-(4-chlorophenyl)-5-(2,4-dichlorophenyl)pyrimidine was prepared from
     2-methylthio-5-(2,4-dichlorophenyl)-4-(4-chlorophenyl)pyrimidine by
     displacement with 4-fluorobenzyl alc. in the presence of NaH in DMF; the
     pyrimidine reactant was prepared by cyclization of pseudothiourea sulfate
     with 3-dimethylamino-1-(4-chlorophenyl)-2-(2,4-dichlorophenyl)prop-2-ene,
     which was prepared by condensation of DMF dimethylacetal with 4-chlorobenzyl
```

2,4-dichlorophenyl ketone, which was prepared from 2,4-dichlorobenzonitrile and a Grignard solution derived from 4-chlorobenzyl bromide. For I: R1 = H, C1-10alkyl, -ORa, -NRaRb, -NRbC(O)Ra, -CO2Ra, -C(O)NRaRb, cyano, -SRb, and -SO2Rb; R2 = H, C1-10alkyl, -ORa, -NRaRb, -NRaC(O)Rb, -CO2Ra, -C(O)NRaRb, cyano, -SRa, and -SO2Ra; R3 = aryl, and heteroaryl, wherein each is (un)substituted with 1-4 Rg; R4 = aryl, and heteroaryl, wherein each is (un)substituted with 1-4 Rg; each Ra = H, C1-10alkyl, C2-10 alkenyl, etc.; each Rb = H, C1-10alkyl, C2-10 alkenyl, cycloalkyl, etc. or Ra and Rb together with the N atom to which they are attached form a bridged or unbridged heterocyclic ring = 4-7 members containing 0-2 addnl. O, S and NRd; each Rg = halogen, C1-10alkyl, -O-C1-4alkyl, -S-C1-4-alkyl, -CN, -CF3, and -OCF3; and m = 1 or 2; addnl. details are given in the claims.

IT 676563-51-2P, 2-(3-Chlorobenzylamino)-4-(2,4-dichlorophenyl)-5-(4-chlorophenyl)pyrimidine

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of substituted pyrimidines for treating disorders mediated by the cannabinoid-1 receptor)

RN 676563-51-2 CAPLUS

CN

2-Pyrimidinamine, 5-(4-chlorophenyl)-N-[(3-chlorophenyl)methyl]-4-(2,4-dichlorophenyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 42 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:264063 CAPLUS

DN 140:423223

TI Combinatorial Synthesis of Substituted Biaryls and Heterocyclic Arylamines

AU Ma, Yao; Margarida, Laura; Brookes, Jeseca; Makara, Gergely M.; Berk, Scott C.

CS NeoGenesis Pharmaceuticals, Inc., Cambridge, MA, 02139, USA

SO Journal of Combinatorial Chemistry (2004), 6(3), 426-430 CODEN: JCCHFF; ISSN: 1520-4766

PB American Chemical Society

DT Journal

LA English

OS CASREACT 140:423223

AB In this paper, we report very general conditions that enable palladium-mediated coupling reactions on the solid support. A wide variety of biaryls and arylamines (including pyrimidines) have been synthesized using this protocol. The chemical facilitates a combinatorial approach to the production of large nos. of medicinally relevant heterocyclic structures.

IT 691858-65-8P 691858-68-1P

RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)

(combinatorial synthesis of substituted biaryls and heterocyclic arylamines via palladium-mediated coupling reactions on a solid support)

RN 691858-65-8 CAPLUS

CN 4-Pyrimidinamine, N-[(4-methylphenyl)methyl]-2-(2-phenoxyphenyl)- (9CI) (CA INDEX NAME)

RN 691858-68-1 CAPLUS

CN 2,4-Pyrimidinediamine, N2,N2-dimethyl-N4-[(4-methylphenyl)methyl]-6-phenyl-(9CI) (CA INDEX NAME)

RE.CNT 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 43 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:205964 CAPLUS

DN 142:74474

TI Product class 12: pyrimidines

AU von Angerer, S.

CS Germany

SO Science of Synthesis (2004), 16, 379-572 CODEN: SSCYJ9

PB Georg Thieme Verlag

DT Journal; General Review-

LA English

AB A review. Methods for preparing pyrimidines are reviewed including cyclization, ring transformation, aromatization and substituent modification.

IT 76990-15-3P 811450-01-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of pyrimidines via cyclization, ring transformation, aromatization and substituent modification)

RN 76990-15-3 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-phenyl-6-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 811450-01-8 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,4-dihydro-4-oxo-2-phenyl-6-[(phenylmethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

RE.CNT 856 THERE ARE 856 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

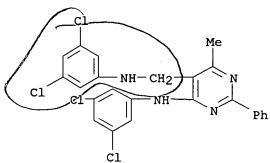
- L10 ANSWER 44 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2004:83424 CAPLUS
- DN 141:314277
- TI Synthesis and antibacterial activity of 1,3-diarylpyrimido[4,5-d]pyrimidines
- AU Cieplik, J.; Pluta, J.; Gubrynowicz, O.
- CS Department of Organic Chemistry, Medical Academy, Wroclaw, Pol.
- SO Bollettino Chimico Farmaceutico (2003), 142(4), 146-150 CODEN: BCFAAI; ISSN: 0006-6648
- PB Societa Editoriale Farmaceutica
- DT Journal
- LA English
- OS CASREACT 141:314277
- AB This paper describes the synthesis of 4,5-diaminoderivatives of pyrimidine and pyrimido[4,5-d]pyrimidines and evaluation of their antibacterial activity on 9 selected bacterial species relating the changes in the chemical structure to an increase in the bioactive properties.
- IT 769141-35-7P 769141-36-8P 769141-37-9P 769141-38-0P 769141-39-1P 769141-40-4P

RL: PAC (Pharmacological activity); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(cyclization of; preparation and antibacterial activity-structure relationships of diarylpyrimidopyrimidines)

RN 769141-35-7 CAPLUS

CN 5-Pyrimidinemethanamine, N-(3,5-dichlorophenyl)-4-[(3,5-dichlorophenyl)amino]-6-methyl-2-phenyl- (9CI) (CA INDEX NAME)





RN 769141-36-8 CAPLUS

CN 5-Pyrimidinemethanamine, N-(3,4-dichlorophenyl)-4-[(3,4-dichlorophenyl)amino]-6-methyl-2-phenyl- (9CI) (CA INDEX NAME)

RN 769141-37-9 CAPLUS

CN 5-Pyrimidinemethanamine, 4-[(3,4-dichlorophenyl)amino]-N-(4-ethoxyphenyl)-6-methyl-2-phenyl- (9CI) (CA INDEX NAME)

RN 769141-38-0 CAPLUS

CN 5-Pyrimidinemethanamine, N-(3,4-dichlorophenyl)-4-[(4-ethoxyphenyl)amino]-6-methyl-2-phenyl- (9CI) (CA INDEX NAME)

RN 769141-39-1 CAPLUS

CN 5-Pyrimidinemethanamine, N-(3,5-dichlorophenyl)-4-[(4-ethoxyphenyl)amino]-6-methyl-2-phenyl- (9CI) (CA INDEX NAME)

RN 769141-40-4 CAPLUS

CN Phenol, 4-[[5-[[(4-chlorophenyl)amino]methyl]-6-methyl-2-phenyl-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)

RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 45 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
     2004:41642 CAPLUS
AN
DN
     140:105256
ΤI
     Antisense oligonucleotides for inhibiting human histone deacetylase 7, 8,
     and 1 expression, benzamide inhibitors of HDAC-7, HDAC-8, and HDAC-1
     isoenzymes, and their use as antitumor agents
     Besterman, Jeffrey M.; Li, Zuomei; Delorme, Daniel; Bonfils, Claire
IN
PA
     Methylgene, Inc., Can.
     PCT Int. Appl., 98 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     English
LА
FAN.CNT 1
     PATENT NO.
                                              APPLICATION NO.
                          KIND
                                 DATE
                                                                      DATE
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PΙ
     WO 2004005513
                           A2
                                 20040115
                                              WO 2003-IB3052
                                                                      20030612
     WO 2004005513
                           Α3
                                 20040701
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT,
             TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     US 2004072770
                           A1
                                 20040415
                                             US 2002-189818
                                                                      20020703
     CA 2490579
                           AA
                                 20040115
                                              CA 2003-2490579
                                                                      20030612
     AU 2003281299
                           A1
                                 20040123
                                              AU 2003-281299
                                                                      20030612
PRAI US 2002-189818
                                 20020703
                           Α
     WO 2003-IB3052
                                 20030612
                           W
AB
     This invention relates to the inhibition of histone deacetylase (HDAC)
     expression and enzymic activity. The invention provides methods and
     reagents for inhibiting HDAC-7 and HDAC-8 by inhibiting expression at the
     nucleic acid level or inhibiting enzymic activity at the protein level.
     Specifically, the invention claims three antisense oligonucleotides and
     benzamide compds. which lead to inhibition of proliferation and cell death
     of contacted cells. The invention further claims chimeric or hybrid
     HDAC-7, HDAC-8, or HDAC-1 antisense oligonucleotides and small mol.
     inhibitors for inhibiting neoplastic cell proliferation in an animal or
     human. Antisense oligonucleotides AS1 and AS2 inhibited HDAC7 mRNA
     expression in human A549 bladder carcinoma cells. AS2 also inhibited
     HDAC8 mRNA expression. An antisense oligonucleotide against HDAC1 acted
     synergistically with HDAC7 and HDAC8 antisense inhibitors to induce
     apoptosis in A549 cells. Small mol. inhibitors of HDAC7 and HDAC8
     together with HDAC1 inhibited human tumor growth in a mouse disease model.
IT
     503043-80-9P, N-(2-Aminophenyl)-4-{[(4-(3,4-dimethoxy-phenyl)-
     pyrimidin-2-ylamino]-methyl}-benzamide
     RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
     study); PREP (Preparation); USES (Uses)
        (antisense oligonucleotides for inhibiting human histone deacetylase 7,
        8, and 1 expression, benzamide inhibitors of HDAC-7, HDAC-8, and HDAC-1
        isoenzymes, and their use as antitumor agents)
RN
     503043-80-9 CAPLUS
CN
     Benzamide, N-(2-aminophenyl)-4-[[[4-(3,4-dimethoxyphenyl)-2-
```

pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)

IT 645401-62-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(benzamide inhibitors of HDAC-7, HDAC-8, and HDAC-1 isoenzymes, and their use as antitumor agents)

RN 645401-62-3 CAPLUS

CN Benzoic acid, 4-[[[4-(3,4-dimethoxyphenyl)-2-pyrimidinyl]amino]methyl]-(9CI) (CA INDEX NAME)

L10 ANSWER 46 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2004:14825 CAPLUS

DN 140:181645

TI New synthesis and biologically active molecular design of deazapteridine-steroid hybrid compounds

AU Nagamatsu, Tomohisa; Yamada, Hiroki; Shiromoto, Kazuyuki

CS Faculty of Pharmaceutical Sciences, Okayama University, Okayama, 700-8530, Japan

SO Heterocycles (2004), 63(1), 9-16 CODEN: HTCYAM; ISSN: 0385-5414

PB Japan Institute of Heterocyclic Chemistry

DT Journal

LA English

OS CASREACT 140:181645

AB This paper describes a facile and general synthesis of a new class of the hybrid compds. possessing a 5-deazapteridine and a steroid unit in the same ring system. These compds. were prepared by condensation of 6-aminouracil derivs. with $(5\alpha,17\beta)-3-(4-\text{morpholinyl})$ and rost-2-en-17-ol or 4,5 α -dihydro-2-(hydroxymethylene) testosterone $[(5\alpha,17\beta)-17$ -hydroxy-2-(hydroxymethylene) and rostan-3-one] under heating in the presence of p-toluenesulfonic acid monohydrate. These compds. are potential anti-coccidiosis agents and some compds. were more active in vitro than robenidine.

IT 66487-67-0, 2-Phenyl-6-[(phenylmethyl)amino]-4(1H)-pyrimidinone
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and biol. active mol. design of deazapteridine-steroid hybrid compds.)

RN 66487-67-0 CAPLUS

CN 4(1H)-Pyrimidinone, 2-phenyl-6-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 47 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
L10
AN
     2004:2818 CAPLUS
DN
     140:59406
ΤI
     Preparation of [[[(hetero)arylamino]methyl]phenoxy]acetic acid derivatives
     as hPPAR activators for treatment of cardiovascular disease and related
IN
     Beswick, Paul John; Harling, John David; Kleanthous, Savvas; Patel,
     Vipulkumar Kantibhai; Simpson, Juliet
PA
     Smithkline Beecham Corporation, USA
SO
     PCT Int. Appl., 98 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                            KIND
                                    DATE
                                                 APPLICATION NO.
                                                                            DATE
                            ----
PΙ
     WO 2004000762
                             A2
                                    20031231
                                                 WO 2003-EP6416
                                                                            20030618
     WO 2004000762
                             A3
                                    20041014
              AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH,
          W:
                                                                                  CN,
              CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
              GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
              LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
              PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT,
          TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2489359
                             AΑ
                                    20031231
                                                 CA 2003-2489359
                                                                            20030618
                                                 AU 2003-245963
     AU 2003245963
                             A1
                                    20040106
                                                                            20030618
     EP 1513795
                             A2
                                    20050316
                                                 EP 2003-738057
                                                                            20030618
              AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     BR 2003011935
                                    20050322
                                                 BR 2003-11935
                             Α
                                                                            20030618
     JP 2005534673
                             T2
                                    20051117
                                                 JP 2004-514762
                                                                            20030618
                                                 NO 2004-5327
     NO 2004005327
                             Α
                                    20050310
                                                                            20041203
     US 2006074111
                             A1
                                    20060406
                                                 US 2004-518778
                                                                            20041217
PRAI GB 2002-14254
                             Α
                                    20020620
     WO 2003-EP6416
                             W
                                    20030618
OS
     MARPAT 140:59406
AB
     Title compds. I [wherein R1 and R2 = independently H or alkyl; X = a bond,
     CH2, or O; R3 and R4 = independently H, alkyl, OCH3, CF3, allyl, or halo;
     X1 = CH2, SO2, or CO; R5 = alkenyl, alkanoyl, alkylsulfonyl, or
     (un) substituted alkyl(phenyl); R6 = (un) substituted Ph or 6-membered
     heteroaryl; or pharmaceutically acceptable salts, solvates, or
     hydrolyzable esters thereof] were prepared as human peroxisome proliferator
     activated receptor (hPPAR) activators. For example, coupling of Et
     2-methyl-2-[2-methyl-4-[[[4-(trifluoromethyl)benzyl]amino]methyl]phenoxy]p
     ropanoate with 2-bromo-6-[4-(trifluoromethyl)phenyl]pyridine in the
     presence of Pd(OAc)2, (R)-2,2'-bis(diphenylphosphino)-1,1'-binaphthyl, and
     cesium carbonate in toluene gave the tertiary amine. Saponification with NaOH
in
     THF provided the acid II. Compds. of the invention showed at least 50%
     activation of hPPAR\delta relative to the pos. control at concns. of 10-7
     M or less. Thus, I and their pharmaceutical compns. are useful for the
     treatment of hPPAR mediated conditions, such as dyslipidemia, syndrome X,
     heart failure, hypercholesterolemia, cardiovascular disease, type II
     diabetes mellitus, type I diabetes, insulin resistance, hyperlipidemia,
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obesity, anorexia bulimia, or anorexia nervosa (no data).
IT
     637353-48-1P, [4-[[Butyl[4-[4-(trifluoromethyl)phenyl]pyrimidin-2-
    yl]amino]methyl]-2-methylphenoxy]acetic acid 637353-49-2P,
     [4-[[Butyl[4-(4-chlorophenyl)pyrimidin-2-yl]amino]methyl]-2-
    methylphenoxy]acetic acid 637353-50-5P, [4-[[(2-Methoxyethyl)[4-
     [4-(trifluoromethyl)phenyl]pyrimidin-2-yl]amino]methyl]-2-
    methylphenoxy] acetic acid 637353-51-6P, [4-[[4-(4-
    Chlorophenyl)pyrimidin-2-yl](2-methoxyethyl)amino]methyl]-2-
    methylphenoxy]acetic acid 637353-52-7p, [2-Methyl-4-[[propyl[4-
     [4-(trifluoromethyl)phenyl]pyrimidin-2-yl]amino]methyl]phenoxy]acetic acid
    637353-70-9P, [4-[[Butyl[5-methyl-6-[4-
     (trifluoromethyl)phenyl]pyrimidin-4-yl]amino]methyl]-2-
    methylphenoxy]acetic acid 637353-71-0P,
     [4-[[Butyl[6-(4-methoxyphenyl)-5-methylpyrimidin-4-yl]amino]methyl]-2-
    methylphenoxy]acetic acid 637353-72-1P, [4-[[Butyl[5-methyl-6-(4-
    methylphenyl)pyrimidin-4-yl]amino]methyl]-2-methylphenoxy]acetic acid
    637353-73-2P, [4-[[Butyl[6-(4-chlorophenyl)-5-methylpyrimidin-4-
    yl]amino]methyl]-2-methylphenoxy]acetic acid 637353-77-6P,
     [2-Methyl-4-[[5-methyl-6-[4-(trifluoromethyl)phenyl]pyrimidin-4-
    yl](propyl)amino]methyl]phenoxy]acetic acid 637353-78-7P,
     [4-[[[6-(4-Chlorophenyl)-5-methylpyrimidin-4-yl](propyl)amino]methyl]-2-
    methylphenoxy]acetic acid 637353-79-8P, [2-Methyl-4-[[[5-methyl-
    6-(4-methylphenyl)pyrimidin-4-yl](propyl)amino]methyl]phenoxy]acetic acid
    637353-80-1P, [2-Methyl-4-[[[5-methyl-6-[4-
     (methyloxy)phenyl]pyrimidin-4-yl](propyl)amino]methyl]phenoxy]acetic acid
    637353-83-4P, [4-[[Butyl[5-methyl-6-(4-methylphenyl)pyrimidin-4-
    yl]amino]methyl]-2-ethylphenoxy]acetic acid 637353-85-6P,
     [4-[[Butyl[6-(4-chlorophenyl)-5-methylpyrimidin-4-yl]amino]methyl]-2-
    ethylphenoxy]acetic acid 637353-86-7P, [4-[[Butyl[5-methyl-6-[4-
     (trifluoromethyl)phenyl]pyrimidin-4-yl]amino]methyl]-2-ethylphenoxy]acetic
    acid 637353-87-8P, [2-Ethyl-4-[[[2-(methyloxy)ethyl][4-[4-
     (trifluoromethyl)phenyl]pyrimidin-2-yl]amino]methyl]phenoxy]acetic acid
    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (hPPAR activator; preparation of [[[(hetero)arylamino]methyl]phenoxy]acetic
       acid derivs. as hPPAR activators for treatment of cardiovascular
       disease and related disorders)
RN
    637353-48-1 CAPLUS
CN
    Acetic acid, [4-[[butyl[4-[4-(trifluoromethyl)phenyl]-2-
    pyrimidinyl]amino]methyl]-2-methylphenoxy}- (9CI) (CA INDEX NAME)
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RN 637353-49-2 CAPLUS
CN Acetic acid, [4-[[butyl[4-(4-chlorophenyl)-2-pyrimidinyl]amino]methyl]-2methylphenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Cl} & \text{Me} \\ \hline & \text{N} & \text{Bu-n} \\ \hline & \text{N-CH}_2 \\ \end{array}$$

RN 637353-50-5 CAPLUS

CN Acetic acid, [4-[[(2-methoxyethyl)[4-[4-(trifluoromethyl)phenyl]-2-pyrimidinyl]amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} F_3C & & CH_2-CH_2-OMe \\ \hline & N & N-R \\ \end{array}$$

RN 637353-51-6 CAPLUS

CN Acetic acid, [4-[[[4-(4-chlorophenyl)-2-pyrimidinyl](2-methoxyethyl)amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

RN 637353-52-7 CAPLUS

CN Acetic acid, [2-methyl-4-[[propyl[4-[4-(trifluoromethyl)phenyl]-2-pyrimidinyl]amino]methyl]phenoxy]- (9CI) (CA INDEX NAME)

F3C
$$N$$
 $Pr-n$ $O-CH_2-CO_2H$ $N-CH_2$

RN 637353-70-9 CAPLUS

CN Acetic acid, [4-[[butyl[5-methyl-6-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

F3C
$$N$$
 N $Bu-n$ $N-CH_2$ $O-CH_2-CO_2H$ Me

RN 637353-71-0 CAPLUS

CN Acetic acid, [4-[[butyl[6-(4-methoxyphenyl)-5-methyl-4-pyrimidinyl]amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

MeO N Bu-n O-CH₂-CO₂H
$$N - CH2$$
Me

RN 637353-72-1 CAPLUS

CN Acetic acid, [4-[[butyl[5-methyl-6-(4-methylphenyl)-4-pyrimidinyl]amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

Me
$$N N Bu-n$$
 $N CH_2$ $N CH_2$

RN 637353-73-2 CAPLUS

CN Acetic acid, [4-[[butyl[6-(4-chlorophenyl)-5-methyl-4-pyrimidinyl]amino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

C1
$$N Bu-n$$
 $N-CH_2$ $N-CH_2$ $N-CH_2$

RN 637353-77-6 CAPLUS

CN Acetic acid, [2-methyl-4-[[[5-methyl-6-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]propylamino]methyl]phenoxy]- (9CI) (CA INDEX NAME)

RN 637353-78-7 CAPLUS

CN Acetic acid, [4-[[[6-(4-chlorophenyl)-5-methyl-4-pyrimidinyl]propylamino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

C1
$$N Pr-n$$
 $N-CH_2$ $N-CH_2$ $N-CH_2$

RN 637353-79-8 CAPLUS

CN Acetic acid, [2-methyl-4-[[[5-methyl-6-(4-methylphenyl)-4-pyrimidinyl]propylamino]methyl]phenoxy]- (9CI) (CA INDEX NAME)

RN 637353-80-1 CAPLUS

CN Acetic acid, [4-[[[6-(4-methoxyphenyl)-5-methyl-4-

pyrimidinyl]propylamino]methyl]-2-methylphenoxy]- (9CI) (CA INDEX NAME)

MeO N Pr-n
$$O-CH_2-CO_2H$$
Me $N-CH_2$

RN 637353-83-4 CAPLUS

CN Acetic acid, [4-[[butyl[5-methyl-6-(4-methylphenyl)-4-pyrimidinyl]amino]methyl]-2-ethylphenoxy]- (9CI) (CA INDEX NAME)

Me N Bu-n
$$O-CH_2-CO_2H$$
Me Me

RN 637353-85-6 CAPLUS

CN Acetic acid, [4-[[butyl[6-(4-chlorophenyl)-5-methyl-4-pyrimidinyl]amino]methyl]-2-ethylphenoxy]- (9CI) (CA INDEX NAME)

C1
$$N N Bu-n$$
 $N-CH_2$ $N-CH_2$

RN 637353-86-7 CAPLUS

CN Acetic acid, [4-[[butyl[5-methyl-6-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]-2-ethylphenoxy]- (9CI) (CA INDEX NAME)

F3C
$$N$$
 N $Bu-n$ $N-CH_2$ $O-CH_2-CO_2H$ Me

RN 637353-87-8 CAPLUS

CN Acetic acid, [2-ethyl-4-[[(2-methoxyethyl)[4-[4-(trifluoromethyl)phenyl]-2-pyrimidinyl]amino]methyl]phenoxy]- (9CI) (CA INDEX NAME)

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IT
     637352-79-5P, Ethyl 2-[4-[[butyl[4-[4-
     (trifluoromethyl)phenyl]pyrimidin-2-yl]amino]methyl]-2-
    methylphenoxy]acetate 637352-80-8P, Ethyl 2-[4-[[butyl[4-(4-
     chlorophenyl)pyrimidin-2-yl]amino]methyl]-2-methylphenoxy]acetate
     637352-81-9P, Ethyl 2-[4-[[(2-methoxyethyl)][4-[4-
     (trifluoromethyl)phenyl]pyrimidin-2-yl]amino]methyl]-2-
    methylphenoxy]acetate 637352-82-0P, Ethyl 2-[4-[[[4-(4-
     chlorophenyl)pyrimidin-2-yl](2-methoxyethyl)amino]methyl]-2-
    methylphenoxy]acetate 637352-83-1P, Ethyl 2-[2-methyl-4-
     [[propyl[4-[4-(trifluoromethyl)phenyl]pyrimidin-2-
     yl]amino]methyl]phenoxy]acetate 637353-01-6P, Ethyl
     2-[4-[[buty1[5-methy1-6-[4-(trifluoromethy1)pheny1]pyrimidin-4-
     yl]amino]methyl]-2-methylphenoxy]acetate 637353-02-7P, Ethyl
     2-[4-[[butyl[6-(4-methoxyphenyl)-5-methylpyrimidin-4-yl]amino]methyl]-2-
     methylphenoxy]acetate 637353-03-8P, Ethyl 2-[4-[[butyl[6-(4-
     chlorophenyl)-5-methylpyrimidin-4-yl]amino]methyl]-2-methylphenoxy]acetate
     637353-04-9P, Ethyl 2-[4-[[butyl[5-methyl-6-(4-
    methylphenyl)pyrimidin-4-yl]amino]methyl]-2-methylphenoxy]acetate
     637353-14-1P, Ethyl 2-[2-methyl-4-[[[5-methyl-6-[4-
     (trifluoromethyl)phenyl]pyrimidin-4-yl](propyl)amino]methyl]phenoxy]acetat
     e 637353-15-2P, Ethyl 2-[4-[[[6-(4-chlorophenyl)-5-
    methylpyrimidin-4-yl](propyl)amino]methyl]-2-methylphenoxy]acetate
     637353-16-3P, Ethyl 2-[2-methyl-4-[[[5-methyl-6-(4-
     methylphenyl)pyrimidin-4-yl](propyl)amino]methyl]phenoxy]acetate
     637353-17-4P, Ethyl 2-[2-methyl-4-[[[5-methyl-6-[4-
     (methyloxy)phenyl]pyrimidin-4-yl](propyl)amino]methyl]phenoxy]acetate
     637353-25-4P, Ethyl 2-[4-[[butyl[5-methyl-6-(4-
     methylphenyl)pyrimidin-4-yl]amino]methyl]-2-ethylphenoxy]acetate
     637353-28-7P, Ethyl 2-[4-[[butyl[6-(4-chlorophenyl)-5-
     methylpyrimidin-4-yl]amino]methyl]-2-ethylphenoxy]acetate
     637353-29-8P, Ethyl 2-[4-[[butyl[5-methyl-6-[4-
     (trifluoromethyl)phenyl]pyrimidin-4-yl]amino]methyl]-2-
     ethylphenoxy]acetate 637353-30-1P, Ethyl 2-[2-ethyl-4-[[[2-
     (methyloxy) ethyl] [4-[4-(trifluoromethyl) phenyl] pyrimidin-2-
     yl]amino]methyl]phenoxy]acetate
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (intermediate; preparation of [[[(hetero)arylamino]methyl]phenoxy]acetic
```

acid derivs. as hPPAR activators for treatment of cardiovascular

disease and related disorders)

RN 637352-79-5 CAPLUS

CN Acetic acid, [4-[[butyl[4-[4-(trifluoromethyl)phenyl]-2-pyrimidinyl]amino]methyl]-2-methylphenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 637352-80-8 CAPLUS

CN Acetic acid, [4-[[butyl[4-(4-chlorophenyl)-2-pyrimidinyl]amino]methyl]-2-methylphenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

C1
$$N = N - CH_2$$
 $N = N - CH_2 - C - OEH_2$

RN 637352-81-9 CAPLUS

CN Acetic acid, [4-[[(2-methoxyethyl)[4-[4-(trifluoromethyl)phenyl]-2-pyrimidinyl]amino]methyl]-2-methylphenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{F3C} & & \text{CH}_2\text{--}\text{CH}_2\text{--}\text{OMe} \\ \hline & & \text{N} & \text{N} \\ \hline & & \text{N} & \text{R} \\ \end{array}$$

RN 637352-82-0 CAPLUS

CN Acetic acid, [4-[[[4-(4-chlorophenyl)-2-pyrimidinyl](2-methoxyethyl)amino]methyl]-2-methylphenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 637352-83-1 CAPLUS

CN Acetic acid, [2-methyl-4-[[propyl[4-[4-(trifluoromethyl)phenyl]-2-pyrimidinyl]amino]methyl]phenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

F₃C
$$N$$
 $Pr-n$ $O-CH_2-C-OEt$

RN 637353-01-6 CAPLUS

CN Acetic acid, [4-[[butyl[5-methyl-6-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]-2-methylphenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

F3C
$$N Bu-n$$
 $O-CH_2-C-OEt$ Me $O-CH_2-C-OEt$

RN 637353-02-7 CAPLUS

CN Acetic acid, [4-[[butyl[6-(4-methoxyphenyl)-5-methyl-4-pyrimidinyl]amino]methyl]-2-methylphenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 637353-03-8 CAPLUS

CN Acetic acid, [4-[[butyl[6-(4-chlorophenyl)-5-methyl-4-pyrimidinyl]amino]methyl]-2-methylphenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 637353-04-9 CAPLUS

CN Acetic acid, [4-[[butyl[5-methyl-6-(4-methylphenyl)-4-pyrimidinyl]amino]methyl]-2-methylphenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

Me N Bu-n O CH₂ C OEt Me N CH₂
$$N - CH_2$$

RN 637353-14-1 CAPLUS

CN Acetic acid, [2-methyl-4-[[[5-methyl-6-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]propylamino]methyl]phenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 637353-15-2 CAPLUS

CN Acetic acid, [4-[[[6-(4-chlorophenyl)-5-methyl-4-pyrimidinyl]propylamino]methyl]-2-methylphenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

C1
$$\begin{array}{c|c}
N & Pr-n \\
N & N-CH_2
\end{array}$$
Me
$$\begin{array}{c|c}
O \\
O-CH_2-C-OEt
\end{array}$$

RN 637353-16-3 CAPLUS

CN Acetic acid, [2-methyl-4-[[[5-methyl-6-(4-methylphenyl)-4-pyrimidinyl]propylamino]methyl]phenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 637353-17-4 CAPLUS

CN Acetic acid, [4-[[[6-(4-methoxyphenyl)-5-methyl-4-pyrimidinyl]propylamino]methyl]-2-methylphenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

MeO
$$N$$
 $Pr-n$ $O-CH_2-C-OET$ $N-CH_2$

RN 637353-25-4 CAPLUS

CN Acetic acid, [4-[[butyl[5-methyl-6-(4-methylphenyl)-4-pyrimidinyl]amino]methyl]-2-ethylphenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

Me
$$N - CH_2$$

Et $O - CH_2 - C - OEt$

Me

RN 637353-28-7 CAPLUS

CN Acetic acid, [4-[[butyl[6-(4-chlorophenyl)-5-methyl-4-pyrimidinyl]amino]methyl]-2-ethylphenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 637353-29-8 CAPLUS

CN Acetic acid, [4-[[butyl[5-methyl-6-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]methyl]-2-ethylphenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

RN 637353-30-1 CAPLUS

CN Acetic acid, [2-ethyl-4-[[(2-methoxyethyl)][4-[4-(trifluoromethyl)phenyl]-2-pyrimidinyl]amino]methyl]phenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{F}_3\text{C} & \text{CH}_2\text{--}\text{CH}_2\text{--}\text{OMe} \\ \hline & \text{N} & \text{N} \text{---}\text{R} \\ \end{array}$$

ANSWER 48 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN L10

AN 2004:2701 CAPLUS

DN 140:53404

ΤI Amino-substituted monocycles as AKT-1 kinase modulators

IN Darrow, James W.; Desimone, Robert W.; Pippin, Douglas A.; Mitchell, Scott

PA Cellular Genomics, Inc., USA

PCT Int. Appl., 43 pp. so

CODEN: PIXXD2

DT Patent

LA English

FAN.	CNT 1															
	PATENT NO.			KIND		DATE			APPLICATION NO.							
PI		2004000318 2004000318				20031231			WO 2003-US19978							
	₩:	AE, AG, CO, CR, GM, HR, LS, LT, PL, PT, UA, UG,	AL, CU, HU, LU, RO,	AM, CZ, ID, LV, RU,	AT, DE, IL, MA, SC,	AU, DK, IN, MD, SD,	AZ, DM, IS, MG, SE,	DZ, JP, MK, SG,	EC, KE, MN, SK,	EE, KG, MW,	ES, KP, MX,	FI, KR, MZ,	GB, KZ, NO,	GD, LC, NZ,	GE, LK, OM,	GH, LR, PH,
	RW:	GH, GM, KG, KZ, FI, FR, BF, BJ,	KE, MD, GB, CF,	LS, RU, GR, CG,	MW, TJ, HU, CI,	MZ, TM, IE, CM,	SD, AT, IT, GA,	SL, BE, LU, GN,	SZ, BG, MC, GQ,	CH, NL, GW,	CY, PT, ML,	CZ, RO, MR,	DE, SE, NE,	DK, SI, SN,	EE, SK, TD,	ES, TR, TG
						2004	0318		US 2003-602560							
PRAI	RAI US 2002-390628P WO 2003-US19978					20020621										
os	OS MARPAT 140:53404															

AΒ A composition comprises amino-substituted monocycle, a pharmaceutically acceptable salt, hydrate, solvate, crystal form, diastereomer, prodrug, or mixture thereof. The compds. are of utility as modulators of kinase activity.

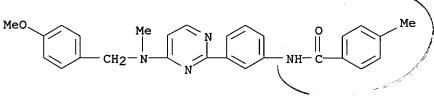
IT 639450-14-9P 639450-15-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(amino-substituted monocycles as AKT-1 kinase modulators)

RN 639450-14-9 CAPLUS

CN Benzamide, N-[3-[4-[[(4-methoxyphenyl)methyl]methylamino]-2pyrimidinyl]phenyl]-4-methyl- (9CI) (CA INDEX NAME)



RN 639450-15-0 CAPLUS

CN Benzamide, 4-methyl-N-[3-[4-[methyl[[4-(trifluoromethyl)phenyl]methyl]amin o]-2-pyrimidinyl]phenyl]- (9CI) (CA INDEX NAME)



IT 639450-14-9D, prodrugs and diastereoisomers 639450-15-0D

, prodrugs and diastereoisomers

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL

(Biological study); USES (Uses)

(amino-substituted monocycles as AKT-1 kinase modulators)

RN 639450-14-9 CAPLUS

CN Benzamide, N-[3-[4-[[(4-methoxyphenyl)methyl]methylamino]-2-pyrimidinyl]phenyl]-4-methyl- (9CI) (CA INDEX NAME)

RN 639450-15-0 CAPLUS

CN Benzamide, 4-methyl-N-[3-[4-[methyl[[4-(trifluoromethyl)phenyl]methyl]amin o]-2-pyrimidinyl]phenyl]- (9CI) (CA INDEX NAME)

```
ANSWER 49 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
     2003:551510 CAPLUS
AN
DN
     139:117434
TI
     Aminopyrimidines as adenosine receptor antagonists, processes for their
     preparation and pharmaceutical compositions
IN
     Tsutsumi, Hideo; Yonishi, Satoshi; Akahane, Atsushi
     Fujisawa Pharmaceutical Co., Ltd., Japan
PA
     PCT Int. Appl., 220 pp.
SO
     CODEN: PIXXD2
\mathbf{DT}
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                          KIND
                                 DATE
                                              APPLICATION NO.
                                                                      DATE
ΡI
     WO 2003057689
                           A1
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                                                                       20021227
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             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LŚ,
             LT, LU, LV, MA, MD, MG, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT,
             RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG,
             US, UZ, VC, VN, YU, ZA, ZM, ZW
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     AU 2002358999
                           A1
                                 20030724
                                              AU 2002-358999
                                                                       20021227
     US 2005043315
                           A1
                                 20050224
                                              US 2004-498016
                                                                       20040616
PRAI AU 2002-9796
                           Α
                                 20020102
     AU 2002-1724
                           Α
                                 20020412
     AU 2002-951403
                                 20020916
                           Α
     WO 2002-JP13796
                           W
                                 20021227
AΒ
     Title compound I [wherein Q = Q1, Q2; R, R4 = (un)substituted aryl,
     heterocyclyl; R5 = H, halogen, alkyl, (un) substituted hydroxy, amino,
     mercapto, alkylsulfinyl, alkylsulfonyl, X = O, S; R1 = H, (un)substituted
     alkyl and cycloalkyl optionally interrupted by an O; R2, R3 =
     independently H, alkyl, acyl, aryl, heterocyclylalkyl; NR2R3 =
     N-heterocyclyl] and their salts were prepared as adenosine receptor
     antagonists. For example, compound II was prepared from 3-(phenylethynyl)-6-
     (phenylsulfonyl)pyridazine in five steps by methanolysis, water addition to
     the triple bond, condensation with N,N-dimethylformamide di-Me acetal,
     cyclocondensation with guanidine hydrochloride and demethylation.
     showed binding to the human Al adenosine receptor with Ki = 11.35 nM and
     to the human A2a adenosine receptor with Ki = 3.85 nM. Thus, I are useful
     as Al receptor and A2a receptor dual antagonists and for the prevention
     and/or treatment of depression, dementia (e.g. Alzheimer's disease,
     cerebrovascular dementia, dementia accompanying Parkinson's disease,
     etc.), Parkinson's disease, anxiety, pain, cerebrovascular disease (e.g.
     stroke, etc.), heart failure and the like (no data).
IT
     560113-07-7P, 6-[2-Amino-4-(benzylamino)-6-phenyl-5-pyrimidinyl]-2-
     isopropyl-3(2H)-pyridazinone 560113-08-8P, 6-[2-Amino-4-
     [benzyl(methyl)amino]-6-phenyl-5-pyrimidinyl]-2-isopropyl-3(2H)-
     pyridazinone 560113-35-1P, 6-[2-Amino-4-(benzylamino)-6-phenyl-5-
     pyrimidinyl]-2-methyl-3(2H)-pyridazinone 560113-50-0P,
     6-[2-Amino-4-(benzylamino)-6-(4-fluorophenyl)-5-pyrimidinyl]-2-isopropyl-
     3(2H)-pyridazinone
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
```

(A1 and A2a adenosine receptor ligand; preparation of aminopyrimidines as adenosine receptor antagonists)

RN 560113-07-7 CAPLUS

CN 3(2H)-Pyridazinone, 6-[2-amino-4-phenyl-6-[(phenylmethyl)amino]-5-pyrimidinyl]-2-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 560113-08-8 CAPLUS

CN 3(2H)-Pyridazinone, 6-[2-amino-4-[methyl(phenylmethyl)amino]-6-phenyl-5-pyrimidinyl]-2-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 560113-35-1 CAPLUS

CN 3(2H)-Pyridazinone, 6-[2-amino-4-phenyl-6-[(phenylmethyl)amino]-5-pyrimidinyl]-2-methyl- (9CI) (CA INDEX NAME)

RN 560113-50-0 CAPLUS

CN 3(2H)-Pyridazinone, 6-[2-amino-4-(4-fluorophenyl)-6-[(phenylmethyl)amino]-5-pyrimidinyl]-2-(1-methylethyl)- (9CI) (CA INDEX NAME)

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 50 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
     2003:417726 CAPLUS
AN
     138:401748
DN
TI
     Preparation of 5-phenylpyrimidines as agricultural fungicides
     Gypser, Andreas; Grote, Thomas; Schwoegler, Anja; Rheinheimer, Joachim;
IN
     Schieweck, Frank; Tormo i Blasco, Jordi; Rose, Ingo; Schaefer, Peter;
     Gewehr, Markus; Grammenos, Wassilios; Mueller, Bernd; Ammermann, Eberhard;
     Strathmann, Siegfried; Lorenz, Gisela; Stierl, Reinhard
     Basf Aktiengesellschaft, Germany
PA
SO
     PCT Int. Appl., 71 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     German
FAN.CNT 1
                                             APPLICATION NO.
                                                                     DATE
     PATENT NO.
                          KIND
                                 DATE
                                             -----
ΡI
     WO 2003043993
                          A1
                                 20030530
                                             WO 2002-EP12807
                                                                     20021115
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             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SC, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT,
             TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
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             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF,
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                                 20030530
                                             CA 2002-2467683
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                          AΑ
                                                                     20021115
     AU 2002352015
                                             AU 2002-352015
                          Α1
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                                             EP 2002-787691
     EP 1448532
                          A1
                                                                     20021115
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     BR 2002014253
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                                             BR 2002-14253
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     CN 1606547
                                 20050413
                                             CN 2002-825535
                                                                     20021115
                          Α
     JP 2005514363
                          T2
                                 20050519
                                             JP 2003-545630
                                                                     20021115
     ZA 2004004835
                          Α
                                 20050620
                                             ZA 2004-4835
                                                                     20040618
PRAI DE 2001-10156279
                          Α
                                 20011119
     WO 2002-EP12807
                          W
                                 20021115
OS
     MARPAT 138:401748
AB
     Title compds. [I; R1, R2 = H, alkyl, haloalkyl, cycloalkyl,
     halocycloalkyl, alkenyl, haloalkenyl, alkynyl, haloalkynyl; or NR1R2 =
     (saturated) (ether-, thio-, sulfoxy-, sulfonyl-interrupted) (R5,
     R6-substituted) ring; R3 = H, halo, cyano, alkyl, haloalkyl, alkoxy,
     haloalkoxy, alkenyloxy, R4 = H, halo, cyano, OH, mercapto, azido, alkyl,
     alkenyl, alkynyl, haloalkyl, alkoxy, alkenyloxy, alkynyloxy, haloalkoxy,
     alkylthio, alkenylthio, alkynylthio, haloalkylthio, ON:CR5R6, CR7:NOR5,
     NR7N:CR5R6, NR5R6, NR7NR5R6, etc.; R5-R7 = H, alkyl, alkenyl, alkynyl,
     haloalkyl, etc.; X = halo, alkyl, alkoxy, haloalkyl; m = 1-5], were prepared
     Thus, NaH in DMF was treated with acetoxime followed by stirring for 1 h
     at 20°-25°. The reaction mixture was treated with 1 g
     [6-chloro-2-methanesulfonyl-5-(2,4,6-trifluorophenyl)pyrimidin-4-yl]-((S)-
     1-trifluoromethylethyl)amine followed by stirring for 14 h at
     20^{\circ}-25^{\circ} to give 0.6 g [6-chloro-2-(N-
     isopropylidienehydrazino)-5-(2,4,6-trifluorophenyl)-pyrimidin-4-yl]-((S)-1-
     trifluoromethylethyl)amine. The latter at 250 ppm gave 93% control of
     Septoria tritici on wheat.
ΙT
     531518-39-5P
```

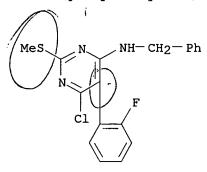
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN

(Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of phenylpyrimidines as agricultural fungicides)

RN 531518-39-5 CAPLUS

CN 4-Pyrimidinamine, 6-chloro-5-(2-fluorophenyl)-2-(methylthio)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 51 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
     2003:301049 CAPLUS
AN
     138:321058
DN
ΤI
     C2-, C6- and 9-Aryl-substituted purine and other heteroaryl kinase
     inhibitor scaffolds and methods for their preparation
     Ding, Sheng; Ding, Qiang; Gray, Nathanael S.
IN
     IRM LLC, Bermuda
PA
     PCT Int. Appl., 68 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     English
LΑ
FAN.CNT 2
     PATENT NO.
                            KIND
                                    DATE
                                                APPLICATION NO.
                                                                            DATE
                            ____
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PΙ
     WO 2003031406
                             A2
                                    20030417
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     WO 2003031406
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                                    20060105
              AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, PR, BY, BZ, CA, CH, CN,
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     CA 2463563
                                    20030417
                                                 CA 2002-2463563
                             AΑ
     US 2003191312
                             A1
                                    20031009
                                                 US 2002-270030
                                                                            20021012
     JP 2005512972
                             T2
                                    20050512
                                                 JP 2003-534390
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                                    20050928
                                                 EP 2002-776216
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                             A2
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     US 2006009642
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                                                 US 2005-223429
                                                                            20050909
PRAI US 2001-328763P
                             Р
                                    20011012
     US 2001-331835P
                            P
                                    20011120
                            Р
     US 2002-346480P
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                            Р
     US 2001-328741P
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     US 2002-346552P
                            Р
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                             Р
     US 2002-347037P
                                    20020108
     US 2002-170031
                             A3
                                    20020612
     WO 2002-US32680
                            W
                                    20021012
     CASREACT 138:321058; MARPAT 138:321058
OS
     General methods for the solution phase as well as solid phase synthesis of
AB
     various substituted heteroaryls, particularly C2-, C6- and
     9-aryl-substituted purines (e.g. 2-(2,4-dimethoxyphenyl)-6-(4-
     methoxybenzylamino)-9-isopropylpurine), was demonstrated. These
     substituted heteroaryls can be further elaborated by aromatic substitution
     with amines at elevated temperature or by anilines, boronic acids and phenols
     via Pd catalyzed cross-coupling reactions. The 1st claim comprises a
     method of preparing a C2-substituted purine compound, said method comprising:
     reacting a C2-halogenated purine with A-X (X = -B(OH)2, -OH, and -NHR1; R1
     = H, (un) substituted alkyl; A = (un) substituted alkyl, (un) substituted
     aryl, (un) substituted heterocyclyl) in the presence of a solvent, a base,
     a carbene ligand and a Pd catalyst. The 2nd claims narrows the 1st claim
     to purines I wherein R2 = H, (un) substituted alkyl, (un) substituted aryl,
     (un) substituted heterocyclyl; X' = direct bond, NR1 and O; X'' = direct bond, O and NR3, with the proviso that when X'' is NR3, Y is R4 or A', and
```

when X' is O or a direct bond, Y is A'; A' = (un)substituted alkyl, (un) substituted aryl, (un) substituted arylalkyl, (un) substituted heterocyclyl; R3 = H, (un)substituted alkyl; and R4 = (un)substituted alkyl. Similar claims pertain to C6-substituted purines. Also claimed is a method of preparing a 9-aryl substituted purines, the method comprising: reacting a 2,6-dihalogenated purine with Ar-B(OH)2 (Ar = (un)substituted aryl, and (un)substituted heterocyclyl) in the presence of a solvent and a Cu catalyst. Also claimed is a method for synthesizing a substituted heteroaryl, the method comprising: providing a dihaloheteroaryl scaffold moiety and capturing the dihaloheteroaryl scaffold moiety on a resin by nucleophilic substitution of a 1st halogen by a resin-bound amine nucleophile to afford a resin-bound amine substituted monohaloheteroaryl. Substitution of the 2nd halogen is done by nucleophilic displacement (e.g. by aniline, phenol, amine, boronic acid) or coupling (e.g. palladium-mediated). An initial substitution (e.g. alkylation, acylation, coupling) can be done prior to substitution of the 1st halogen. Example procedures are included for: boronic acid coupling, aniline coupling, phenol coupling, purine N9 arylation via boronic acids/cupric acetate, reductive amination for synthesis of PAL-resin-bound amine, resin capture of dichloroheterocycles, substitution of remaining chloro group with boronic acids via Suzuki coupling and product cleavage, substitution of remaining chloro group with anilines or amines via palladium-catalyzed reaction and product cleavage, substitution of remaining chloro group with phenols via palladium-catalyzed reaction and product cleavage, substitution of remaining chloro group with amines via non-palladium-catalyzed amination reaction without base and product cleavage, and substitution of remaining chloro group with amines via non-palladium-catalyzed amination reaction with KOtBu as base and product cleavage. Tables of purity and yields for various heteroaryl combinatorial libraries are included as validation of the following methods: palladium catalyzed cross-coupling reactions for derivatizing resin-bound 2-chloro-6-aminopurine with boronic acids, anilines, amines and phenols, resin-bound chloroheterocyclic scaffolds which can be derivatized via Suzuki coupling reaction, resin-bound chloroheterocyclic scaffolds which can be derivatized via palladium catalyzed amination reaction, and resin-bound chloroheterocyclic scaffolds which can be derivatized via palladium catalyzed C-O bond formation reaction. 406932-41-0P, 4-(4-Methoxybenzylamino)-2-(3methoxyphenyl)pyrimidine 406932-42-1P, 4-(4-Methoxybenzylamino)-2-(3-methoxyphenyl)-5-methylpyrimidine 406932-43-2P, 4-(4-Methoxybenzylamino)-2-(3-methoxyphenyl)-6-methylpyrimidine **406932-44-3P**, 4-(4-Methoxybenzylamino)-6-(3methoxyphenyl)pyrimidine 406932-45-4P, 4-(4-Methoxybenzylamino)-6-(3-methoxyphenyl)pyrimidin-2-amine RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation) (C2-, C6- and 9-Aryl-substituted purine and other heteroaryl kinase

ΤT

RN

CN

406932-41-0 CAPLUS

(CA INDEX NAME)

Page 485

4-Pyrimidinamine, 2-(3-methoxyphenyl)-N-[(4-methoxyphenyl)methyl]- (9CI)

inhibitor scaffolds and methods for their preparation)

RN 406932-42-1 CAPLUS

CN 4-Pyrimidinamine, 2-(3-methoxyphenyl)-N-[(4-methoxyphenyl)methyl]-5-methyl-(9CI) (CA INDEX NAME)

RN 406932-43-2 CAPLUS

CN 4-Pyrimidinamine, 2-(3-methoxyphenyl)-N-[(4-methoxyphenyl)methyl]-6-methyl-(9CI) (CA INDEX NAME)

RN 406932-44-3 CAPLUS

CN 4-Pyrimidinamine, 6-(3-methoxyphenyl)-N-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{MeO} & \text{N} & \text{N} \\ \hline & \text{NH-CH}_2 \\ \hline \end{array}$$

RN 406932-45-4 CAPLUS

CN 2,4-Pyrimidinediamine, 6-(3-methoxyphenyl)-N4-[(4-methoxyphenyl)methyl]-

(9CI) (CA INDEX NAME)

```
ANSWER 52 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     2003:261678 CAPLUS
DN
     138:287691
TI
     Preparation of 4-aminopyrimidine derivatives as insulin secretion
     accelerators
IN
     Yonetoku, Yasuhiro; Maruyama, Tatsuya; Negoro, Kenji; Moritomo, Hiroyuki;
     Imanishi, Naoki; Shimada, Itsuro; Moritomo, Ayako; Hamaguchi, Wataru;
     Misawa, Hana; Yoshida, Shigeru; Ohishi, Takahide
PA
     Yamanouchi Pharmaceutical Co., Ltd., Japan
SO
     PCT Int. Appl., 82 pp.
     CODEN: PIXXD2
DΤ
     Patent
LΑ
     Japanese
FAN.CNT 1
     PATENT NO.
                          KIND
                                 DATE
                                             APPLICATION NO.
                                                                      DATE
PΙ
     WO 2003026661
                          A1
                                 20030403
                                             WO 2002-JP9350
                                                                      20020912
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             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,
             LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL,
             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
             UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
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PRAI JP 2001-279671
                           Α
                                 20010914
     JP 2002-121012
                           Α
                                 20020423
os
     MARPAT 138:287691
AB
     Disclosed are insulin secretion accelerators containing the 4-aminopyrimidine
     derivs. [I; R11 = A11-D11 (wherein A11 = single bond, lower alkylene,
     lower alkenylene; D11 = each (un)substituted aryl, cycloalkyl, or aromatic or
     non-aromatic heterocyclyl); R12 = H, lower alkyl optionally substituted by
     ≥1 groups selected from aryl, halo, lower alkoxy, and OH; R13 = H,
     Me, F; R14 = H, lower alkyl optionally substituted by ≥1 halogens;
     R15 = A15-D15 (wherein A15 = single bond, lower alkylene, lower
     alkenylene; D15 = H, lower alkoxy, amino optionally substituted by 1 or 2
     groups selected from lower alkyl and aryl, each (un)substituted aryl,
     cycloalkyl, or aromatic or non-aromatic heterocyclyl)] or pharmaceutically
     acceptable salts thereof as the active ingredients. These compds. are
     highly effective in promoting insulin secretion, increasing insulin
     content, and inhibiting blood sugar level from increasing and are usable
     for treatments for insulin-dependent diabetes, non-insulin-dependent
     diabetes, insulin-resistant diseases, and obesity. Thus, a mixture of 284
     mg 2-(4-bromophenyl)-4-chloro-6-methylpyrimidine, 1 mL 70% aqueous ethylamine
     solution, 2 mL MeOH was stirred at room temperature for 2 h and at 60^{\circ} for 3
     h, treated again with 1 mL 70% aqueous ethylamine solution, and stirred at
     60° for 5 h to give 198 mg N-[2-(4-bromophenyl)-6-methylpyrimidin-4-
     yl]ethylamine (II). II in vitro promoted the secretion of insulin in
     mouse spleen \beta-cells by 159% vs. 122% for Glibenclamide.
IT
     504401-70-1P 504401-72-3P 504401-74-5P
     504401-76-7P 504401-78-9P 504401-80-3P
     504401-82-5P 504401-84-7P 504401-86-9P
     504401-88-1P 504401-90-5P 504401-91-6P
     504401-93-8P 504401-95-0P 504402-60-2P
     504403-06-9P 504403-07-0P
```

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 4-aminopyrimidine derivs. as insulin secretion accelerators for treating diabetes, insulin-resistant diseases, and obesity)

RN 504401-70-1 CAPLUS

4-Pyrimidinamine, 2-(4-bromophenyl)-6-ethyl-N-(phenylmethyl)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CN

CRN 504401-69-8 CMF C19 H18 Br N3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 504401-72-3 CAPLUS

CN 4-Pyrimidinamine, 2-(4-bromophenyl)-6-ethyl-N-[(4-fluorophenyl)methyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 504401-71-2 CMF C19 H17 Br F N3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 504401-74-5 CAPLUS

CN 4-Pyrimidinamine, 2-(4-bromophenyl)-6-ethyl-N-[(4-methylphenyl)methyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 504401-73-4 CMF C20 H20 Br N3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 504401-76-7 CAPLUS

CN 4-Pyrimidinamine, 2-(4-bromophenyl)-6-ethyl-N-[(4-methoxyphenyl)methyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 504401-75-6 CMF C20 H20 Br N3 O

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN504401-78-9 CAPLUS 4-Pyrimidinamine, 2-(4-bromophenyl)-6-ethyl-N-(2-phenylethyl)-, ethanedioate (1:1) (9CI) (CA INDEX NAME) CN

CM1

CRN 504401-77-8 CMF C20 H20 Br N3

$$\begin{array}{c|c} & \text{Et} & \\ & N & \\ \text{Ph-CH}_2\text{-CH}_2\text{-NH} & N & \\ \end{array}$$

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN504401-80-3 CAPLUS 4-Pyrimidinamine, 2-(4-bromophenyl)-6-ethyl-N-[2-(4-fluorophenyl)ethyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME) CN

CM 1

CRN 504401-79-0 CMF C20 H19 Br F N3

$$\begin{array}{c} \text{Br} \\ \text{N} \\ \text{N} \\ \text{NH-CH}_2\text{-CH}_2 \\ \end{array}$$

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 504401-82-5 CAPLUS
CN 4-Pyrimidinamine, 2-(4-bromophenyl)-N-[2-(4-chlorophenyl)ethyl]-6-ethyl-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 504401-81-4 CMF C20 H19 Br Cl N3

CM 2

CRN 144-62-7 CMF C2 H2 O4

CRN 504401-83-6 CMF C20 H19 Br2 N3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 504401-86-9 CAPLUS
CN 4-Pyrimidinamine, 2-(4-bromophenyl)-6-ethyl-N-[2-(4-methylphenyl)ethyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 504401-85-8 CMF C21 H22 Br N3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 504401-88-1 CAPLUS

CN Phenol, 4-[2-[[2-(4-bromophenyl)-6-ethyl-4-pyrimidinyl]amino]ethyl]-, ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 504401-87-0 CMF C20 H20 Br N3 O

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 504401-90-5 CAPLUS

CN 4-Pyrimidinamine, 2-(4-bromophenyl)-6-ethyl-N-[2-(2-methoxyphenyl)ethyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 504401-89-2 CMF C21 H22 Br N3 O

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 504401-91-6 CAPLUS

CN 4-Pyrimidinamine, 2-(4-bromophenyl)-N-[2-(4-methoxyphenyl)ethyl]-6-methyl-(9CI) (CA INDEX NAME)

RN 504401-93-8 CAPLUS

CN 4-Pyrimidinamine, 2-(4-bromophenyl)-6-ethyl-N-[2-(4-methoxyphenyl)ethyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 504401-92-7 CMF C21 H22 Br N3 O

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 504401-95-0 CAPLUS
CN 4-Pyrimidinamine, 2-(4-bromophenyl)-6-ethyl-N-(3-phenylpropyl)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 504401-94-9 CMF C21 H22 Br N3

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 504402-60-2 CAPLUS

CN 8-Quinolineethanamine, N-[2-(4-bromophenyl)-6-methyl-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 504403-06-9 CAPLUS

CN 4-Pyrimidinamine, N-(1,3-benzodioxol-5-ylmethyl)-2-(3-chloro-4-fluorophenyl)-6-ethyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & N & NH-CH_2 \\ \hline & N & Et \\ \end{array}$$

RN 504403-07-0 CAPLUS

CN Phenol, 4-[2-[[2-(3-chloro-4-fluorophenyl)-6-ethyl-4-pyrimidinyl]amino]ethyl]- (9CI) (CA INDEX NAME)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 53 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
     2003:242160 CAPLUS
AN
DN
     138:271705
ΤI
     Preparation of triazinyl and other carboxamides as inhibitors of histone
     deacetylase
IN
     Delorme, Daniel; Woo, Soon Hyung; Vaisburg, Arkadii; Moradel, Oscar; Leit,
     Silvana; Raeppel, Stephane; Frechette, Sylvie; Bouchain, Giliane
PA
     Methylgene, Inc., Can.
so
     PCT Int. Appl., 347 pp.
     CODEN: PIXXD2
DT
     Patent
     English
LА
FAN.CNT 3
     PATENT NO.
                         KIND
                                DATE
                                             APPLICATION NO.
                                                                     DATE
                         ____
                                _____
PΙ
     WO 2003024448
                          A2
                                 20030327
                                             WO 2002-US29017
                                                                     20020912
     WO 2003024448
                          A3
                                 20031113
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF,
             CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2465978
                                 20030327
                                             CA 2002-2465978
                          AA
                                                                     20020912
     EP 1429765
                                             EP 2002-763627
                          A2
                                 20040623
                                                                     20020912
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
     BR 2002012510
                                 20040824
                                             BR 2002-12510
                          Α
                                                                     20020912
                                             CN 2002-822690
     CN 1578663
                          Α
                                 20050209
                                                                     20020912
     JP 2005508905
                          T2
                                 20050407
                                             JP 2003-528544
                                                                     20020912
                                             JP 2005-80310
     JP 2005255683
                          A2
                                20050922
                                                                     20050318
PRAI US 2001-322402P
                          Р
                                20010914
     US 2002-391728P
                          Ρ
                                20020626
     JP 2003-528544
                          A3
                                20020912
     WO 2002-US29017
                          W
                                20020912
OS
     MARPAT 138:271705
     The invention relates to triazines (shown as I; variables defined below;
AB
     e.g. 4-[[4-amino-6-(2-indanylamino)-[1,3,5]triazin-2-ylamino]methyl]-N-(2-
     aminophenyl)benzamide) and Cy3-X1-Ar2-(C(R5):C(R6))qC(O)NH-Ay2 (II;
     variables defined below; e.g. ), many of which are N-(o-
     aminophenyl) carboxamides, as inhibitors of histone deacetylase (data
     included for many I and II). The invention provides compds. and methods
     for inhibiting histone deacetylase enzymic activity. The invention also
     provides compns. and methods for treating cell proliferative diseases and
     conditions. Antineoplastic effects of some I and II are illustrated for
     colorectal, pulmonary and pancreatic neoplasms; also the combined
     antineoplastic effect of histone deacetylase inhibitors and histone
     deacetylase antisense oligonucleotides on tumor cells in vivo was
     demonstrated. For I: R3 and R4 = H, L1, Cyl and -L1-Cyl (L1 = C1-C6
     alkyl, C2-C6 heteroalkyl, or C3-C6 alkenyl; Cy1 = cycloalkyl, aryl,
     heteroaryl, or heterocyclyl) or R3 and R4 are taken together with the
     adjacent N atom to form a 5-, 6-, or 7-membered ring, wherein the ring
     atoms = C, O, S, and N, and wherein the ring is optionally substituted,
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and optionally forms part of a bicyclic ring system, or is optionally

fused to one or two aryl or heteroaryl rings, or to one or two saturated or partially unsatd. cycloalkyl or heterocyclic rings, each of which rings and ring systems is optionally substituted. Y1 = -N(R1)(R2), -CH2-C(0)-N(R1)(R2), halogen, and H (R1 and R2 = H, L1, Cy1, and -L1-Cy1). Y2 = chemical bond or N(R0) (R0 = H, alkyl, aryl, aralkyl, and acyl); Ak1 =C1-C6 alkylene, C1-C6-heteroalkylene (preferably, in which one -CH2- is replaced with -NH-, and more preferably -NH-CH2), C2-C6 alkenylene or C2-C6 alkynylene; Ar1 = arylene or heteroarylene, either of which is optionally substituted; and Z1 = C(0)NH-Ay1 and CH:CHC(0)NH-Ay1 (Ay1 = aryl or heteroaryl, each of which is optionally substituted). For II: Cy2 = cycloalkyl, aryl, heteroaryl, or heterocyclyl; X1 = covalent bond, M1-L2-M1, and L2-M2-L2 (L2 = chemical bond, C1-C4 alkylene, C2-C4 alkenylene, and C2-C4 alkynylene, provided that L2 is not a chemical bond when X1 is M1-L2-M1; M1 = -O-, -N(R7)-, -S-, -S(O)-, S(O)2-, -S(O)2N(R7)-, -N(R7)S(O)2-, -C(O)-, -C(O)NH-, -NHC(O)-, -NHC(O)-O- and -OC(O)NH- (R7 = H, alkyl, aryl, aralkyl, acyl, heterocyclyl, and heteroaryl); and M2 = M1, heteroarylene, and heterocyclylene, either of which rings is optionally substituted). Ar2 = arylene or heteroarylene, each of which is optionally substituted; R5 and R6 = H, alkyl, aryl, and aralkyl; q is 0 or 1; and Ay2 is a 5-6 membered cycloalkyl, heterocyclyl, or heteroaryl substituted with an amino or hydroxy moiety (preferably these groups are ortho to the amide N to which Ay2 is attached) and further optionally substituted; provided that when Cy2 is naphthyl, X1 is -CH2-, Ar2 is Ph, R5 and R6 are H, and q is 0 or 1, Ay2 is not Ph or o-hydroxyphenyl. Although the methods of preparation are not claimed, hundreds of example prepns. are included. 503043-79-6P, N-(2-Aminophenyl)-4-(((4-chloro-6-(3,4-

503043-79-6P, N-(2-Aminophenyl)-4-(((4-chloro-6-(3,4-dimethoxyphenyl)pyrimidin-2-yl)amino)methyl)benzamide 503043-80-9P
, N-(2-Aminophenyl)-4-(((4-(3,4-dimethoxyphenyl)pyrimidin-2-yl)amino)methyl)benzamide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of triazinyl and other carboxamides as inhibitors of histone deacetylase for treating cell proliferative disorders)

RN 503043-79-6 CAPLUS

IT

CN

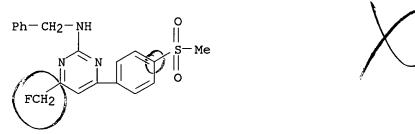
Benzamide, N-(2-aminophenyl)-4-[[[4-chloro-6-(3,4-dimethoxyphenyl)-2-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)

RN 503043-80-9 CAPLUS

CN Benzamide, N-(2-aminophenyl)-4-[[[4-(3,4-dimethoxyphenyl)-2-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)

```
ANSWER 54 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
L10
AN
     2003:133247 CAPLUS
DN
     138:187783
ΤI
     Pyrimidin-2-amines as selective inhibitors of COX-2
IN
     Carter, Malcolm Clive; Naylor, Alan; Payne, Jeremy John; Pegg, Neil
PA
     Glaxo Group Limited, UK
     PCT Int. Appl., 27 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                   DATE
     _____
                                            _____
     WO 2003014091
                                            WO 2002-GB3601
                                                                   20020805
PΙ
                          A1
                                20030220
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
            PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
            CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
            PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
            NE, SN, TD, TG
                                20040506
                                            EP 2002-747620
     EP 1414807
                          A1
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
     JP 2005501086
                          Т2
                                20050113
                                            JP 2003-519041
                                                                   20020805
                                            US 2004-486001
     US 2004248916
                          A1
                                20041209
                                                                   20040729
     US 7056928
                          B2
                                20060606
PRAI GB 2001-19477
                                20010809
                          Α
     WO 2002-GB3601
                          W
                                20020805
os
    MARPAT 138:187783
AB
     The title compds. I [R1, R2 = H, alkyl; R3 = alkyl, NH2, R6CONH; R4 = H,
     alkyl; R5 = CH2F, CHF2, CF3CH2, CF3CHF, CF3CF2; A = (un)substituted 5-6
     membered aryl; R6 = H, alkyl, alkoxy, etc.; n = 0-4] which are potent and
     selective inhibitors of COX-2, and are of use in the treatment of the
     pain, fever, inflammation of a variety of conditions and diseases, were
     prepared E.g., a general procedure for synthesis of II which showed IC50 of
     22 nM against COX-2 vs. IC50 of 17,700 nM against COX-1, was given.
IT
     497943-83-6P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (preparation of pyrimidin-2-amines as selective inhibitors of COX-2 for
        treating inflammatory disorders)
RN
     497943-83-6 CAPLUS
CN
     2-Pyrimidinamine, 4-(fluoromethyl)-6-[4-(methylsulfonyl)phenyl]-N-
```

(phenylmethyl) - (9CI) (CA INDEX NAME)



RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/671,070

L10 ANSWER 55 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2003:98255 CAPLUS

DN 138:287627

TI Suzuki Cross-Coupling of Solid-Supported Chloropyrimidines with Arylboronic Acids

AU Wade, Janice V.; Krueger, Clinton A.

CS ChemRx Division, Discovery Partners International Inc., South San Francisco, CA, 94080, USA

SO Journal of Combinatorial Chemistry (2003), 5(3), 267-272 CODEN: JCCHFF; ISSN: 1520-4766

PB American Chemical Society

DT Journal

LA English

OS CASREACT 138:287627

AB The utility of the Suzuki cross-coupling to synthesize biaryl compds. is expanded herein to include reactions of resin-supported chloropyrimidines with boronic acids. In particular, an efficient method is described for the synthesis of a library of biaryl compds. from solid-supported chloropyrimidines. The Suzuki reaction was performed in an inert atmospheric using Pd2(dba)3/P(t-Bu)3 as catalyst, spray-dried KF as base, and THF as solvent. The reaction was allowed to proceed overnight at 50 °C. Upon cleavage with acid, a library of 4-(substituted amino)-6-arylpyrimidines, e.g. I, was obtained in moderate yield and high purity.

IT 503610-78-4DP, resin-supported 503610-80-8DP,

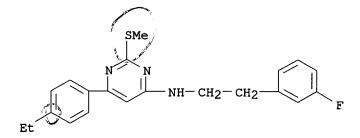
resin-supported

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(Suzuki cross-coupling of solid-supported chloropyrimidines with arylboronic acids)

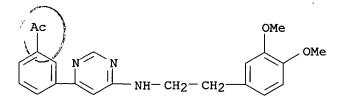
RN 503610-78-4 CAPLUS

CN 4-Pyrimidinamine, 6-(4-ethylphenyl)-N-[2-(3-fluorophenyl)ethyl]-2-(methylthio)- (9CI) (CA INDEX NAME)



RN 503610-80-8 CAPLUS

CN Ethanone, 1-[3-[6-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]- (9CI) (CA INDEX NAME)



IT 503610-78-4P 503610-80-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

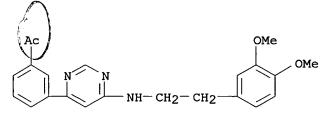
(Suzuki cross-coupling of solid-supported chloropyrimidines with arylboronic acids)

RN 503610-78-4 CAPLUS

CN 4-Pyrimidinamine, 6-(4-ethylphenyl)-N-[2-(3-fluorophenyl)ethyl]-2-(methylthio)- (9CI) (CA INDEX NAME)

RN 503610-80-8 CAPLUS

CN Ethanone, 1-[3-[6-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-4-pyrimidinyl]phenyl]- (9CI) (CA INDEX NAME)



RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 56 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
L10
AN
     2002:977601 CAPLUS
DN
     138:55972
ΤI
     Preparation of pyrimidine inhibitors of phosphodiesterase (PDE) 7
     Guo, Junqing; Barbosa, Joseph; Pitts, William John; Carlsen, Marianne;
IN
     Quesnelle, Claude; Dodier, Marco
PA
     Bristol-Myers Squibb Company, USA
SO
     PCT Int. Appl., 165 pp.
     CODEN: PIXXD2
     Patent
DТ
LΑ
     English
FAN.CNT 7
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                   DATE
                         ____
     ______
                                _____
                                            _____
PΙ
    WO 2002102313
                          A2
                                20021227
                                            WO 2002-US19097
                                                                    20020617
                         A3
                                20030403
    WO 2002102313
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             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
            UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB,
             GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA,
             GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2450934
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                                20021227
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                                                                   20020617
    US 2003162802
                                20030828
                                            US 2002-173442
                          A1
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    EP 1397142
                          A2
                                20040317
                                            EP 2002-744381
                                                                   20020617
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     JP 2005500294
                          Т2
                                20050106
                                            JP 2003-504902
                                                                   20020617
                                            US 2005-281246
     US 2006116516
                          A1
                                20060601
                                                                   20051117
PRAI US 2001-299287P
                         Р
                                20010619
    US 2002-355141P
                          Р
                                20020208
    US 2002-368752P
                          Ρ
                                20020329
    US 2002-173322
                         A3
                                20020617
    WO 2002-US19097
                         W
                                20020617
OS
    MARPAT 138:55972
AB
     The title compds. [I; R1 = H, alkyl; R2 = (un)substituted heteroaryl,
    heterocyclyl, aryl, aryl fused to heteroaryl or heterocyclyl; Z = halo,
    alkyl, aryl, etc.; J = H, halo, alkyl, etc.; L = H, halo, haloalkyl,
     etc.], phosphodiesterase 7 (PDE 7) inhibitors (including both selective
     inhibitors of PDE 7, and dual inhibitors of PDE 7 and phosphodiesterase 4)
    which are useful in treating T-cell mediated diseases, were prepared E.g.,
     a multi-step synthesis of II, starting from 2-imino-4-thiobiuret and Et
     2-chloroacetoacetate, was given.
IT
     479230-18-7P 479230-36-9P 479230-49-4P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (preparation of pyrimidine inhibitors of phosphodiesterase (PDE) 7)
RN
     479230-18-7 CAPLUS
CN
     5-Thiazolecarboxylic acid, 4-methyl-2-[[4-[[[4-
     (methylsulfonyl)phenyl]methyl]amino]-6-(3,4,5-trimethoxyphenyl)-2-
```

pyrimidinyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 479230-36-9 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[4-(4-cyanophenyl)-6-[[[4-(methylsulfonyl)phenyl]methyl]amino]-2-pyrimidinyl]amino]-4-methyl-, ethyl ester (9CI) (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 479230-49-4 CAPLUS

CN 5-Thiazolecarboxylic acid, 2-[[4-[[[4-(aminosulfonyl)phenyl]methyl]amino]-6-(4-carboxyphenyl)-2-pyrimidinyl]amino]-4-methyl-, 5-ethyl ester (9CI) (CA INDEX NAME)

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

```
ANSWER 57 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
L10
AN
      2002:927411 CAPLUS
DN
      138:14068
ΤI
      Preparation of methylsulfonylphenylpyrimidines as cyclooxygenase-2
      inhibitors.
IN
      Green, Richard Howard; Bravi, Gianpaolo; Carter, Malcolm; Hartley, Charles
      David; Naylor, Alan; Pass, Martin; Payne, Jeremy John; Pegg, Neil Anthony
PA
      Glaxo Group Limited, UK; Green, Jennifer Margaret
SO
      PCT Int. Appl., 35 pp.
      CODEN: PIXXD2
DT
      Patent
      English
LА
FAN.CNT 1
      PATENT NO.
                             KIND
                                                   APPLICATION NO.
                                     DATE
                                                                              DATE
                             ____
                                     -----
                                                  -----
PΙ
     WO 2002096886
                              A1
                                     20021205
                                                  WO 2002-GB2408
                                                                              20020523
     WO 2002096886
                              C1
                                     20040722
          W:
              AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
               CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
          PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, CM, CO, CM, MI, MB, ME, SM, TD, TC
               GN, GQ, GW, ML, MR, NE, SN, TD, TG
     EP 1390352
                              A1
                                     20040225
                                                 EP 2002-738325
                                                                              20020523
              AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
               IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     JP 2004532264
                              Т2
                                     20041021
                                                   JP 2003-500065
                                                                              20020523
PRAI GB 2001-12803
                              Α
                                     20010525
     WO 2002-GB2408
                              W
                                     20020523
OS
     MARPAT 138:14068
     Title compds. [I; R1, R2 = H, A, fluoroalkyl, alkenyl, alkynyl,
AΒ
     cycloalkylalkyl, bridged cycloalkyl, X(CR7R8)n, B(CR7R8)n; R3 = A, NH2,
     R10CONH; R4 = fluoroalkyl; R5 = H, A, fluoroalkyl, halo, cycloalkylalkyl;
     when R6 = H, then R5 \neq H; R6 = H, A, fluoroalkyl, halo, alkoxy, CN,
     NO2, AOCO, NH2CO, ANHCO, NH2, ANH, A2N, A2NCO, ACONH, NH2SO2, ANHSO2
     A2NSO2, ASO2NH, ArSO2NH, ASO2, ArSO2, alkenyl, alkynyl; when R5 = H then
     R6 \neq H; R7, R8 = H, A; X = unsubstituted 5- or 6-membered
     heteroaryl, unsubstituted 6-membered aryl, 5- or 6-membered heteroaryl,
     6-membered aryl substituted by ≥1 R9; R9 = OH, halo, A,
     fluoroalkyl, alkoxy, fluoroalkoxy, NH2SO2, ASO2; B = oxetanyl,
     tetrahydrofuryl, tetrahydropyranyl, etc.; R10 = H, A, alkoxy, AOA, Ph,
     HO2CA, AOCOA, AOCO, H2NA, AOCONHA, ACONHA; A = alkyl], were prepared Thus,
     5-methyl-2-(methylsulfonyl)-4-[4-(methylsulfonyl)phenyl]-6-
     (trifluoromethyl)pyrimidine (preparation given) was stirred with PhCH2NH2 in
     1-methyl-2-pyrrolidinone overnight at room temperature to give
     N-benzyl-5-methyl-4-[4-(methylsulfonyl)phenyl]-6-
     (trifluoromethyl)pyrimidin-2-amine. This at 10 μM gave 61% inhibition
     of human cyclooxygenase-2.
IT
     477770-88-0P, N-Benzyl-5-methyl-4-[4-(methylsulfonyl)phenyl]-6-
     (trifluoromethyl)pyrimidin-2-amine 477770-90-4P
     477770-92-6P 477771-01-0P 477771-02-1P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
```

(preparation of methylsulfonylphenylpyrimidines as cyclooxygenase-2 inhibitors)

RN 477770-88-0 CAPLUS

CN 2-Pyrimidinamine, 5-methyl-4-[4-(methylsulfonyl)phenyl]-N-(phenylmethyl)-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 477770-90-4 CAPLUS

CN Phenol, 2-[[[5-methyl-4-[4-(methylsulfonyl)phenyl]-6-(trifluoromethyl)-2-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)

RN 477770-92-6 CAPLUS

CN 2-Pyrimidinamine, 5-methyl-N-[(4-methylphenyl)methyl]-4-[4-(methylsulfonyl)phenyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 477771-01-0 CAPLUS

CN 2-Pyrimidinamine, N-[(4-methoxyphenyl)methyl]-5-methyl-4-[4-(methylsulfonyl)phenyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 477771-02-1 CAPLUS

CN 2-Pyrimidinamine, N-[(4-fluorophenyl)methyl]-5-methyl-4-[4-(methylsulfonyl)phenyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$F$$
 CH_2
 NH
 $S-Me$
 Me

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 58 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
     2002:927396 CAPLUS
AN
     138:13955
DN
TI
     Preparation of phenol and hydroxynaphthalene based inhibitors of protein
     kinase for the treatment of disease
     Cao, Sheldon Xiaodong; Bounaud, Pierre-Yves; Chen, Xiaohua; Chung,
IN
     Hyun-Ho; Dumas, David Paul; Kc, Sunil Kumar; Min, Changhee; Yang, Jae
     Young; Long, Mellissa C.
     LG Biomedical Institute, USA
PA
SO
     PCT Int. Appl., 286 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                     DATE
ΡI
     WO 2002096867
                          A2
                                20021205
                                            WO 2002-US16920
                                                                     20020528
     WO 2002096867
                                20040304
                          А3
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
         W:
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, UZ, VN, YU, ZA, ZM, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB,
             GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     AU 2002310187
                          A1
                                20021209
                                            AU 2002-310187
                                                                     20020528
     US 2003187007
                          A1
                                20031002
                                            US 2002-158030
                                                                     20020528
     US 2003208067
                          A1
                                20031106
                                             US 2002-158103
                                                                     20020528
     EP 1412327
                          A2
                                20040428
                                             EP 2002-737248
                                                                    20020528
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     JP 2004534779
                          T2
                                20041118
                                             JP 2003-500047
                                                                     20020528
PRAI US 2001-294792P
                          Ρ
                                20010530
     WO 2002-US16920
                                20020528
                          W
OS
     MARPAT 138:13955
AB
     Phenol and hydroxynaphthalene derivs. I [X = O, S, amine, alkylamine,
     alkynylamine, arylamine, and heteroarylamine; R1 = (un)substituted 5- or
     6-membered aromatic or heteroarom. ring, -(X1)mCOX2-, wherein X1 = alkylene,
     alkenylene, alkynylene, aryl and heteroaryl, X2 = H, alkyl, aryl,
     heteroaryl, OH, alkoxy, amino, substituted amine, m = 0 or 1, or R1 =
     -C(X3)=N-NX4-C(=E)-NX5X6 wherein X3=H, alkyl, aryl, alkylaryl,
     heteroaryl, and amino and E = 0, S, and substituted amine with X4, X5, and
     X6 independently equal to H, alkyl, aryl, and heteroaryl; R2, R3, and R4 =
     H, alkyl, alkylene, halo, alkoxy, etc.; or R2 and R3 or R3 and R4 may be
     taken together to form an (un) substituted aromatic or heteroarom. ring; R5 =
     H, (un)substituted-alkyl, -aryl, -heterocycle, etc.; R6 = H, alkyl,
     alkene, alkyne, aryl, and heteroaryl] are prepared and disclosed as
     inhibitors of protein kinase. Thus, II was prepared by cyclocondensation of
     5'-bromo-2'-methoxyacetophenone with N,N-dimethylformamide di-Et acetal
     with subsequent Suzuki coupling with 4-methoxyphenylboronic acid. In
     assays to determine cyclin dependent kinase activity, specifically against CDK2
     and CDK5, II possessed IC50 values of 0-0.5 μM. II proved highly
     specific for CDK2 and CDK5 and was further evaluated by in vitro tumor
```

cell efficacy tests against numerous cancers. The present invention is directed in part towards methods of modulating the function of protein

kinases with phenol- and hydroxynaphthalene-based compds. The methods incorporate cells that express a protein kinase. In addition, the invention describes methods of preventing and treating protein kinase-related abnormal conditions in organisms with a compound identified by the invention. Furthermore, the invention pertains to phenol- and hydroxynaphthalene-based compds. and pharmaceutical compns. comprising these compds.

IT 477727-17-6P 477727-24-5P 477727-25-6P 477727-26-7P 477727-27-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of phenol and hydroxynaphthalene based inhibitors of protein kinase)

RN 477727-17-6 CAPLUS

CN [1,1'-Biphenyl]-4,4'-diol, 3-[2-amino-6-[([1,1'-biphenyl]-2-ylmethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 477727-24-5 CAPLUS

CN [1,1'-Biphenyl]-4,4'-diol, 3-[2-amino-6-[[(3-fluorophenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 477727-25-6 CAPLUS

CN [1,1'-Biphenyl]-4,4'-diol, 3-[2-amino-6-[[(2-fluorophenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN- 477727-26-7 CAPLUS

CN [1,1'-Biphenyl]-4,4'-diol, 3-[2-amino-6-[[(3-methoxyphenyl)methyl]amino]-4-

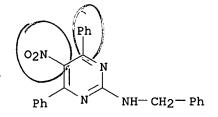
pyrimidinyl] - (9CI) (CA INDEX NAME)

RN 477727-27-8 CAPLUS

CN [1,1'-Biphenyl]-4,4'-diol, 3-[2-amino-6-[[(4-methoxyphenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

10/671,070

- L10 ANSWER 59 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2002:864729 CAPLUS
- DN 138:238120
- TI Synthesis of 2-amino- and 2-hydrazino-substituted 5-nitro-4,6-diphenylpyrimidines
- AU Sedova, V. F.; Shkurko, O. P.; Nekhoroshev, S. A.
- CS Novosibirsk N. N. Vorozhtsov Institute of Organic Chemistry, Siberian Branch, Russian Academy of Sciences, Novosibirsk, 630090, Russia
- SO Chemistry of Heterocyclic Compounds (New York, NY, United States) (Translation of Khimiya Geterotsiklicheskikh Soedinenii) (2002), 38(5), 564-570
 - CODEN: CHCCAL; ISSN: 0009-3122
- PB Kluwer Academic/Consultants Bureau
- DT Journal
- LA English
- OS CASREACT 138:238120
- AB Nitrogen-containing derivs. of 5-nitro-4,6-diphenylpyrimidine have been synthesized by the reaction of 2-chloro-5-nitro-4,6-diphenylpyrimidine with amines or of 2-hydrazino-5-nitro-4,6-diphenylpyrimidine with carbonyl or β -dicarbonyl compds. Their structures were confirmed by IR spectroscopy and mass spectrometry.
- IT 502159-40-2P
 - RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and spectra of amino- and hydrazino-substituted nitrodiphenylpyrimidines from reaction of pyrimidine derivs. with amine and (di)carbonyl compds.)
- RN 502159-40-2 CAPLUS
- CN 2-Pyrimidinamine, 5-nitro-4,6-diphenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



2 P'86

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L10 ANSWER 60 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2002:814853 CAPLUS
- DN 137:325431
- TI Preparation of aminopyrimidines and -pyridines as glycogen synthase kinase 3 inhibitors
- IN Nuss, John M.; Harrison, Stephen D.; Ring, David B.; Boyce, Rustum S.; Johnson, Kirk; Pfister, Keith B.; Ramurthy, Savithri; Seely, Lynn; Wagman, Allan S.; Desai, Manjo; Levine, Barry H.
- PA USA
- SO U.S. Pat. Appl. Publ., 134 pp., Cont.-in-part of U.S. 6,417,185. CODEN: USXXCO
- DT Patent
- LA English
- FAN.CNT 3

	PATENT NO.		KIND	DATE	API	PLICATION NO.	DATE	
PI	US	2002156087	A1	20021024	US	2001-949035	20010906	
	US	7045519	B2	20060516				
	US	6417185	B1	20020709	US	1999-336038	19990618	
	US	2003130289	A 1	20030710	US	2002-309535	20021203	
	US	7037918	B2	20060502				
	US	2006089369	A1	20060427	US	2005-220400	20050906	
PRAI	US	1998-89978P	P	19980619				
	US	1999-336038	A2	19990618				
	US	2000-230480P	P	20000906				
	US	1999-336098	A 3	19990618				
	US	2001-949035	A3	20010906				
		105 005 101						

- OS MARPAT 137:325431
- AΒ Title compds. I [wherein W = (un)substituted C or N; X and Y = independently N, O, or (un) substituted C; A = (un) substituted (hetero) aryl; R1, R1a, R2, R2a, R3, R3a, R4, and R4a = independently H, OH, alkoxy, acyl, (hetero)aryl, or (un)substituted (cyclo)alkyl, amino(alkyl), etc.; R5 and R7 = independently H, halo, alkoxy, guanidinyl, (bi)aryl, hetero(bi)aryl, heterocycloalkyl, arylsulfonamido, or (un)substituted (cyclo)alkyl, amino(alkoxy), or amidino; R6 = H, halo, carboxyl, NO2, (cyclo)amido, (cyclo)amidino, (cyclo)imido, CN, alkoxy, acyl(oxy), guanidinyl, (hetero)aryl, heterocyclo(alkyl), arylsulfonyl, arylsulfonamido, or (un)substituted alkyl, amino, etc.] were prepared as glycogen synthase kinase 3 (GSK3) inhibitors. For example, 2-chloro-5-nitropyridine was aminated by H2N(CH2)3NH2 and the product N-acylated by benzotriazolecarboxamidinium tosylate to give the alkylquanidine. The latter was cyclocondensed with resin-bound 4-(MeCO)C6H4CONHCH2C6H4Br-3 and Cs2CO3 to afford, after resin cleavage, the pyrimidinamine II. The most preferred compds. of the invention exhibited inhibitory activity against human GSK3B in a cell free assay with IC50 values of $< 1 \mu M$. Thus, I and compns. containing I may be employed alone or in combination with other pharmacol. active agents in the treatment of disorders mediated by GSK3 activity, such as diabetes, Alzheimer's disease and other neurodegenerative disorders, obesity, atherosclerotic cardiovascular disease, essential hypertension, polycystic ovary syndrome, syndrome X, ischemia, traumatic brain injury, bipolar disorder, immunodeficiency, or cancer (no data).
- IT 252904-40-8P, Benzonitrile, 4-[2-[[2-[(5-nitro-2pyridinyl)amino]ethyl]amino]-5-[(phenylmethyl)amino]-4-pyrimidinyl]RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(preparation of aminopyrimidines and -pyridines as glycogen synthase kinase

3 inhibitors)
RN 252904-40-8 CAPLUS
CN Benzonitrile, 4-[2-[[2-[(5-nitro-2-pyridinyl)amino]ethyl]amino]-5[(phenylmethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

Ph-CH2-NH

IT **403806-74-6**, 4-[2-[[(3-Methylphenyl)methyl]amino]pyrimidin-4yl]benzamide 403806-75-7, 4-[2-[[(4-Aminophenyl)methyl]amino]pyrimidin-4-yl]benzamide 403806-80-4, 4-[2-[[(4-Cyanophenyl)methyl]amino]pyrimidin-4-yl]benzamide **403806-81-5**, 4-[2-[[(3-Methoxyphenyl)methyl]amino]pyrimidin-4yl]benzamide 403806-82-6, 4-[2-[[(4-Methoxyphenyl)methyl]amino]pyrimidin-4-yl]benzamide 403806-83-7, 4-[2-[[2-(4-Fluorophenyl)ethyl]amino]pyrimidin-4-yl]benzamide 403806-87-1, 4-[2-[[(3-Chlorophenyl)methyl]amino]pyrimidin-4yl]benzamide 403806-92-8, 4-[2-[(4-Phenylbutyl)amino]pyrimidin-4yl]benzamide 403806-94-0, 4-[2-[[2-(3-Methoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzamide 403806-98-4, 4-[2-[[(3-Nitrophenyl)methyl]amino]pyrimidin-4-yl]benzamide **403807-02-3**, 4-[2-[[2-(3-Chlorophenyl)ethyl]amino]pyrimidin-4yl]benzamide 403807-03-4, 4-[2-[(Naphthylmethyl)amino]pyrimidin-4-y1]benzamide 403807-07-8, 4-[2-[[2-(2,5-Dimethoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzenecarbonitrile 403807-11-4, 4-[2-[[2-(2H-Benzo[3,4-d]-1,3-dioxolan-5yl)ethyl]amino]pyrimidin-4-yl]benzamide 403807-12-5, 4-[2-[[2-(4-Nitrophenyl)ethyl]amino]pyrimidin-4-yl]benzamide 403807-13-6, 4-[2-[[(2,6-Dimethoxyphenyl)methyl]amino]pyrimidin-4yl]benzamide 403807-14-7, 4-[2-[[(3,4-Dimethoxyphenyl)methyl]amino]pyrimidin-4-yl]benzamide 403807-19-2 , 4-[2-[[[3-(Trifluoromethyl)phenyl]methyl]amino]pyrimidin-4-yl]benzamide 403807-20-5, 4-[2-[[[4-(Trifluoromethyl)phenyl]methyl]amino]pyrimi din-4-yl]benzamide 403807-21-6, 4-[2-[[(3,5-Dichlorophenyl)methyl]amino]pyrimidin-4-yl]benzamide 403807-23-8 , 4-[2-[((2,4-Dichlorophenyl)methyl]amino]pyrimidin-4-yl]benzamide 403807-37-4, 4-[2-[[(4-Bromophenyl)methyl]amino]pyrimidin-4yl]benzamide 403807-38-5, 4-[2-[[[4-(4-

```
Fluorophenyl)phenyl]methyl]amino]pyrimidin-4-yl]benzamide
     403807-39-6, 4-[2-[[(3-Bromophenyl)methyl]amino]pyrimidin-4-
     yl]benzamide 403807-47-6, 4-[2-[[(3,4,5-
    Trimethoxyphenyl)methyl]amino]pyrimidin-4-yl]benzamide 403807-49-8
     , 4-[2-[[[3-(3-Aminophenyl)phenyl]methyl]amino]pyrimidin-4-yl]benzamide
     403807-50-1, 4-[2-[[[4-(3-Aminophenyl)phenyl]methyl]amino]pyrimidi
    n-4-y1]benzamide 403807-53-4, Ethyl 4-(4-cyanophenyl)-2-[[2-(3-
    methoxyphenyl)ethyl]amino]pyrimidine-5-carboxylate 403807-60-3,
     4-[2-[[[3-(3-Methoxyphenyl)phenyl]methyl]amino]pyrimidin-4-yl]benzamide
     403807-65-8, 4-[2-[[[3-[3-[(Methylamino)methyl]phenyl]phenyl]methy
     l]amino]pyrimidin-4-yl]benzamide 403807-78-3,
     4-[2-[[[3-[3-(Acetylamino)phenyl]phenyl]methyl]amino]pyrimidin-4-
     yl]benzamide 403807-79-4, 4-[2-[[[3,5-
     Bis(trifluoromethyl)phenyl]methyl]amino]pyrimidin-4-yl]benzamide
     403807-83-0, 4-[2-[[[3-[3-(Trifluoromethyl)phenyl]phenyl]methyl]am
     ino]pyrimidin-4-yl]benzamide 403808-16-2, [4-[2-[[(3-
     Bromophenyl) methyl] amino] pyrimidin-4-yl] phenyl] -N-[(3-
    methylphenyl)methyl]carboxamide 403808-32-2,
    N-[(3-Bromophenyl)methyl]-4-[2-[[2-(3-methoxyphenyl)ethyl]amino]pyrimidin-
     4-yl]phenylcarboxamide 403808-46-8 403809-22-3,
     4-[2-[[2-(2,5-Dimethoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzamide
     403809-23-4, 4-[2-[[2-(2,3-Dimethoxyphenyl)ethyl]amino]pyrimidin-4-
     yl]benzamide 403810-50-4
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (preparation of aminopyrimidines and -pyridines as glycogen synthase kinase
        3 inhibitors)
RN
     403806-74-6 CAPLUS
CN
     Benzamide, 4-[2-[[(3-methylphenyl)methyl]amino]-4-pyrimidinyl]- (9CI)
                                                                             (CA
    INDEX NAME)
H<sub>2</sub>N
                       NH-CH2
RN
     403806-75-7 CAPLUS
CN
     Benzamide, 4-[2-[[(4-aminophenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA
     INDEX NAME)
                      NH-CH2
RN
     403806-80-4 CAPLUS
CN
     Benzamide, 4-[2-[[(4-cyanophenyl)methyl]amino]-4-pyrimidinyl]- (9CI)
                                                                            (CA
```

INDEX NAME)

$$H_2N-C$$
 N
 $N+CH_2$
 N

RN 403806-81-5 CAPLUS

CN Benzamide, 4-[2-[[(3-methoxyphenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ H_2N-C \\ \hline \\ N \\ \end{array} \begin{array}{c} N \\ NH-CH_2 \\ \hline \\ OMe \\ \end{array}$$

RN 403806-82-6 CAPLUS

CN Benzamide, 4-[2-[[(4-methoxyphenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \mathsf{C} & \mathsf{C} & \mathsf{C} \\ \mathsf{H}_2\mathsf{N}-\mathsf{C} & \mathsf{N} & \mathsf{N}\mathsf{H}-\mathsf{C}\mathsf{H}_2 \\ \hline & \mathsf{N} & \mathsf{N}\mathsf{H}-\mathsf{C}\mathsf{H}_2 \\ \end{array}$$

RN 403806-83-7 CAPLUS

CN Benzamide, 4-[2-[[2-(4-fluorophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \circ & \\ \parallel & & \\ H_2N-C & & \\ \hline & N & NH-CH_2-CH_2 \end{array}$$

RN 403806-87-1 CAPLUS

CN Benzamide, 4-[2-[[(3-chlorophenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \circ \\ \parallel \\ \text{H}_2\text{N}-\text{C} \\ \hline \\ N \\ \end{array}$$
 NH- CH₂

RN 403806-92-8 CAPLUS

CN Benzamide, 4-[2-[(4-phenylbutyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 403806-94-0 CAPLUS

CN Benzamide, 4-[2-[[2-(3-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ H_2N-C & & & \\ \hline & N & NH-CH_2-CH_2 \\ \hline \end{array}$$

RN 403806-98-4 CAPLUS

CN Benzamide, 4-[2-[[(3-nitrophenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$H_2N-C$$
 N
 $NH-CH_2$
 $NO2$

RN 403807-02-3 CAPLUS

CN Benzamide, 4-[2-[[2-(3-chlorophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 403807-03-4 CAPLUS

CN Benzamide, 4-[2-[(1-naphthalenylmethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 403807-07-8 CAPLUS

CN Benzonitrile, 4-[2-[[2-(2,5-dimethoxyphenyl)ethyl]amino]-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{OMe} \\ \\ \text{NC} \end{array}$$

RN 403807-11-4 CAPLUS

CN Benzamide, 4-[2-[[2-(1,3-benzodioxol-5-yl)ethyl]amino]-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O \\ H_2N-C \\ \hline \\ N \\ \end{array} \qquad NH-CH_2-CH_2 \\ \hline \\ O \\ O \\ \end{array}$$

RN 403807-12-5 CAPLUS

CN Benzamide, 4-[2-[[2-(4-nitrophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$H_2N-C$$
 N
 $NH-CH_2-CH_2$

RN 403807-13-6 CAPLUS

CN Benzamide, 4-[2-[[(2,6-dimethoxyphenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ H_2N-C & \\ \hline \\ N & \\ NH-CH_2 \\ \hline \\ OMe \\ \end{array}$$

RN 403807-14-7 CAPLUS

CN Benzamide, 4-[2-[[(3,4-dimethoxyphenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & OMe \\ H_2N-C & N \\ \hline & N \\ \hline & NH-CH_2 \\ \hline \end{array}$$

RN 403807-19-2 CAPLUS

CN Benzamide, 4-[2-[[[3-(trifluoromethyl)phenyl]methyl]amino]-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

$$H_2N-C$$
 N
 $NH-CH_2$
 CF_3

RN 403807-20-5 CAPLUS

CN Benzamide, 4-[2-[[[4-(trifluoromethyl)phenyl]methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$H_2N-C$$
 N
 $N+CH_2$
 CF_3

RN 403807-21-6 CAPLUS

CN Benzamide, 4-[2-[[(3,5-dichlorophenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} 0 \\ \parallel \\ \parallel \\ 1 \\$$

RN 403807-23-8 CAPLUS

CN Benzamide, 4-[2-[[(2,4-dichlorophenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 403807-37-4 CAPLUS

CN Benzamide, 4-[2-[[(4-bromophenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 403807-38-5 CAPLUS

CN Benzamide, 4-[2-[[(4'-fluoro[1,1'-biphenyl]-4-yl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & & \\ H_2N-C & & & & \\ \hline & N & NH-CH_2 & & \\ \end{array}$$

RN 403807-39-6 CAPLUS

CN Benzamide, 4-[2-[[(3-bromophenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 403807-47-6 CAPLUS

CN Benzamide, 4-[2-[[(3,4,5-trimethoxyphenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ H_2N-C & & & \\ & & & \\ O & & & \\ \end{array} \begin{array}{c} OMe \\ OMe \\ \end{array}$$

RN 403807-49-8 CAPLUS

CN Benzamide, 4-[2-[[(3'-amino[1,1'-biphenyl]-3-yl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ H_2N-C & & & \\ \hline & N & NH-CH_2 & & \\ \hline & NH_2 & & \\ \end{array}$$

RN 403807-50-1 CAPLUS

CN Benzamide, 4-[2-[[(3'-amino[1,1'-biphenyl]-4-yl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \circ \\ \vdots \\ h_2 n - c \\ \hline \\ N \\ \end{array} \\ \begin{array}{c} N \\ N + C \\ h_2 \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\ N \\ \end{array} \\ \begin{array}{c} N \\ N \\$$

RN 403807-53-4 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-2-[[2-(3-methoxyphenyl)ethyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 403807-60-3 CAPLUS

CN Benzamide, 4-[2-[[(3'-methoxy[1,1'-biphenyl]-3-yl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 403807-65-8 CAPLUS

CN Benzamide, 4-[2-[[[3'-[(methylamino)methyl][1,1'-biphenyl]-3-yl]methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O \\ C-NH_2 \end{array}$$

$$MeNH-CH_2 \\ \hline \end{array}$$

RN 403807-78-3 CAPLUS

CN Benzamide, 4-[2-[[[3'-(acetylamino)[1,1'-biphenyl]-3-yl]methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 403807-79-4 CAPLUS

CN Benzamide, 4-[2-[[[3,5-bis(trifluoromethyl)phenyl]methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & \\ H_2N-C & & & & & & \\ \hline & & & & & & \\ N & & & NH-CH_2 & & & \\ \hline & & & & & \\ CF_3 & & & & \\ \end{array}$$

RN 403807-83-0 CAPLUS

CN Benzamide, 4-[2-[[[3'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$_{\mathrm{F_{3}C}}$$

RN 403808-16-2 CAPLUS

CN Benzamide, 4-[2-[[(3-bromophenyl)methyl]amino]-4-pyrimidinyl]-N-[(3-methylphenyl)methyl]- (9CI) (CA INDEX NAME)

$$Br$$
 CH_2-NH N $C-NH-CH_2$ Me

RN 403808-32-2 CAPLUS

CN Benzamide, N-[(3-bromophenyl)methyl]-4-[2-[[2-(3-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 403808-46-8 CAPLUS

CN Benzamide, N-[(3-bromophenyl)methyl]-4-[2-[[2-(2,5-dimethoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 403809-22-3 CAPLUS

CN Benzamide, 4-[2-[[2-(2,5-dimethoxyphenyl)ethyl]amino]-4-pyrimidinyl](9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ \parallel \\ H_2N-C \\ \hline \\ N \\ NH-CH_2-CH_2 \\ \hline \\ OMe \\ \\ OMe \\ \end{array}$$

RN 403809-23-4 CAPLUS

CN Benzamide, 4-[2-[[2-(2,3-dimethoxyphenyl)ethyl]amino]-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O \\ H_2N-C \\ \hline \\ N \\ \hline \\ NH-CH_2-CH_2 \\ \hline \\ OMe \\ \hline \\ OMe \\ \end{array}$$

RN 403810-50-4 CAPLUS
CN Benzamide, 4-[2-[[2-(2-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI)
(CA INDEX NAME)

$$\begin{array}{c|c} \mathsf{N} & \mathsf{MeO} \\ \mathsf{N} & \mathsf{NH-CH_2-CH_2} \end{array}$$

RE.CNT 306 THERE ARE 306 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 61 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
L10
AN
     2002:777933 CAPLUS
DN
     137:294969
ΤĮ
     4-Aryl-substituted 2-pyrimidinamines and 2-pyridinamines, useful as
     inhibitors of c-Jun N-terminal kinases (JNK) and other protein kinases
     Bethiel, Randy; Cochran, John; Moon, Young-Choon; Nanthakumar, Susanthini
IN
PΑ
     Vertex Pharmaceuticals Incorporated, USA
     PCT Int. Appl., 115 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LА
     English
FAN.CNT 1
                                           APPLICATION NO.
     PATENT NO.
                        KIND
                               DATE
                                                                   DATE
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                                           -----
                                                                   _____
PΙ
    WO 2002079197
                         A1
                               20021010
                                           WO 2002-US9554
                                                                   20020328
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            GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
            LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
            PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
            UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,
            TJ, TM
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,
            CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
            BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2441733
                               20021010
                                           CA 2002-2441733
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                         AΑ
                                20030508
     US 2003087922
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    US 6949544
                                20050927
                         B2
                                           EP 2002-725391
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                                20040102
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            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     JP 2004529140
                         T2
                               20040924
                                           JP 2002-577822
                                                                   20020328
PRAI US 2001-279961P
                         Ρ
                                20010329
     WO 2002-US9554
                         W
                                20020328
     MARPAT 137:294969
AB
     The invention provides compds. of formula I and II, and their
     pharmaceutically acceptable derivs. [wherein: W = N, CH; R1, R2, R3 = halo,
     QR, QnCN, QnNO2, QnAr2; or R1R2, R2R3 = 4- to 8-membered (un)saturated ring
     with 0-3 N/O/S atoms; n = 0 or 1; Q = C1-4 alkylidene with one CH2
     optionally replaced by O, S, NR, NRCO, CO, CO2, CONR, SO2, SO2NR, NRSO2NR,
     etc.; R = H, (un) substituted aliphatic; or NRR = 3- to 7-membered (un) saturated
     ring with 1-2 addnl. N/O/S atoms; R4 = Ar1, TAr2, TnAr3; T = C1-2
     alkylidene with optional replacement of a CH2 as above; Ar1 =
     (un) substituted 5- to 6-membered mono- or bicyclic (un) saturated ring system;
     Ar2 = (un) substituted 5- to 6-membered (un) saturated monocyclic ring with 0-3
     N/O/S atoms, or (un)substituted 8- to 10-membered (un)saturated bicyclic ring
     with 0-5 N/O/S atoms; Ar3 = 6-membered aryl with 0-2 N atoms and
     substituted with certain groups; with provisos and exclusions].
     compds. are inhibitors of protein kinases, particularly JNK, a mammalian
     protein kinase involved in cell proliferation, cell death and response to
     extracellular stimuli. Furthermore, they are inhibitors of Src-family
     kinases, especially Src and Lck kinases. The compds. are also inhibitors of
     GSK3 and CDK2 kinases. The invention also relates to methods for
     producing the compds. Also provided are pharmaceutical compns. comprising
     I or II, and methods of utilizing those compns. in the treatment and
     prevention of various disorders. Three tables of approx. 240 compds. were
     prepared and claimed., and most were tested against at least one of the five
```

mentioned kinases. For instance, 3,4-dihydroxy-5-methoxybenzaldehyde was

cyclized with 1,2-dibromoethane to give a benzodioxane derivative, followed by elaboration of the formyl group to Me2NCH:CH:CO- in 3 steps. Cyclization of the resultant enaminone with 3-chlorophenylguanidine gave title compound III. This compound inhibited cloned human JNK3 protein in vitro with Ki < 0.1 μ M.

IT 468084-56-2P, 4-(3,4,5-Trimethoxyphenyl)-N-(phenylmethyl)-2-pyrimidinamine

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of phenyl-substituted pyridinamines and pyrimidinamines as inhibitors of c-Jun N-terminal kinases (JNK) and other protein kinases)

RN 468084-56-2 CAPLUS

CN 2-Pyrimidinamine, N-(phenylmethyl)-4-(3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/671,070

L10 ANSWER 62 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2002:565745 CAPLUS

DN 138:39247

TI Microwave-assisted synthesis of aminopyrimidines

AU Luo, Guanglin; Chen, Ling; Poindexter, Graham S.

CS Department of Chemistry, Bristol-Myers Squibb Pharmaceutical Research Institute, Wallingford, CT, USA

SO Tetrahedron Letters (2002), 43(33), 5739-5742 CODEN: TELEAY; ISSN: 0040-4039

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 138:39247

AB Series of mono- or di-substituted aminopyrimidine derivs. were synthesized through microwave-assisted aromatic nucleophilic substitution or Suzuki coupling.

IT 266303-86-0P, 4-Benzylamino-6-phenylpyrimidine
RL: SPN (Synthetic preparation); PREP (Preparation)
 (microwave-assisted aromatic nucleophilic substitution or Suzuki coupling preparation of aminopyrimidines)

RN 266303-86-0 CAPLUS

CN 4-Pyrimidinamine, 6-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT



L10 ANSWER 63 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2002:546802 CAPLUS

DN 138:221538

TI Reactions with 6-phenyl-2-thiouracil and preparation of substituted and fused pyrimidine derivatives

AU Al-Haiza, Mohammed A.

CS Chemistry Department, College of Science, King Khalid University, Abha, Saudi Arabia

SO Journal of Saudi Chemical Society (2002), 6(1), 71-81 CODEN: JSCSFO; ISSN: 1319-6103

PB Saudi Chemical Society

DT Journal

LA English

OS CASREACT 138:221538

AB Alkylation of 6-phenyl-2-thiouracil (1) gave the S-alkyl derivs. 2a,b. Compound 2a could also be prepared by a different method via the reaction of S-methylisothiourea with Et benzoylacetate. Desulphurization of 2a with hydrazine yielded the 2-hydrazino derivative 3, which condensed with aromatic aldehydes to produce the Schiff's bases 4a-c. The reaction of 3 with each of carbon disulfide and nitrous acid resulted in the formation of s-triazolo[4,3-a]- and tetrazolo[1,5-a]pyrimidine derivs. 5 and 7, resp. Treatment of 2a,b with phosphorus oxychloride formed the 4-chloropyrimidine derivs. 11a,b. Compds. 11a,b reacted the thiophenol, benzylamine, hydrazine, anthranilic acid and Et anthranilate to give the trisubstituted pyrimidine derivs. 12a-e. Compound 12d was obtained by the hydrolysis of its ester derivative 12e, since the reaction of anthranilic acid with 11a produced directly the pyrido[6,1-b]quinazoline 13. The latter compound could also be synthesized via an alternative route by cyclization of compound 12d. Similarly, the reaction of glycine with 11a afforded directly imidazo[1,2c]pyrimidine 14. Moreover, the reaction of the dihydrazinopyrimidine derivative 12c with each of carbon disulfide and nitrous acid formed the ditriazolo[4,3-a:4,3 -c]- and the ditetrazolo[1,5-:1,5 -c]pyrimidines 15 and 16, resp. Compound 1 reacted with 1,3-dichloroacetone to give compound 17. Oxidation of 1 afforded the expected disulfide product

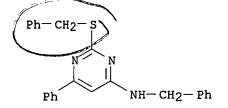
IT 501030-18-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(in preparation of substituted and fused pyrimidine derivs. from 6-phenylthiouracil)

RN 501030-18-8 CAPLUS

CN 4-Pyrimidinamine, 6-phenyl-N-(phenylmethyl)-2-[(phenylmethyl)thio]- (9CI) (CA INDEX NAME)





RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 64 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
     2002:220583 CAPLUS
AN
     136:247583
DN
ΤI
     Preparation of pyrazolamines and analogs as protein kinase inhibitors for
     treatment of cancer, diabetes, and Alzheimer's disease
     Davies, Robert; Bebbington, David; Knegtel, Ronald; Wannamaker, Marion;
IN
     Li, Pan; Forester, Cornelia; Pierce, Albert; Kay, David
     Vertex Pharmaceuticals Incorporated, USA
PA
     PCT Int. Appl., 373 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     English
LA
FAN.CNT 14
     PATENT NO.
                          KIND
                                             APPLICATION NO.
                                                                      DATE
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PΙ
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             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,
             PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,
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     BR 2001014088
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     EP 1318997
                          A1
                                 20030618
                                             EP 2001-971082
     EP 1318997
                          В1
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             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     ZA 2003001701
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     ZA 2003001703
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                                             ZA 2003-1703
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     JP 2004509117
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                                                                     20011219
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     EP 1345922
                          A1
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                                             EP 2001-271061
                                                                     20011219
     EP 1345922
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AB Title compds. I [wherein G = Ring C or Ring D; Ring C = (un)substituted Ph, pyridinyl, pyrimidinyl, pyridazinyl, pyrazinyl, or 1,2,4-triazinyl;

Ring D = (un)substituted monocyclic or bicyclic ring selected from aryl, heteroaryl, heterocyclyl, or carbocyclyl; Z1 = N or CR9; Z2 = N or CH; Z3 = N or CRx; Z4 = N or CRy; Rx and Ry = independently TR3, or taken together with their intervening atoms form an (un) saturated fused ring having 1-3 ring heteroatoms; R2 and R2a = independently R, TWR6; or C2R2R2a = (un) substituted fused ring containing 0-3 heteroatoms; T = a bond or alkylidene chain; W = C(R6)2O, C(R6)2SO-2, C(R6)2NR6, CO, CO2, CR6OCO, CR60CONR6, C(R6) 2NR6CO, C(R6) 2NR6CO2, CR6:NNR6, CR6:NO, C(R6) 2NR6NR6, C(R6) 2NR6SO2NR6, C(R6) 2NR6CONR6, or CONR6; R = H or (un) substitutedaliphatic, (hetero)aryl, or heterocyclyl ring; R3 = R, halo, O, OR, COR, CO2R, COCOR, COCH2COR, NO2, CN, SO0-2R, N(R4)2, CON(R4)2, SO2N(R4)2, OCOR, NR4COR, NR4CO2(aliphatic), NR4N(R4)2, C:NN(R4)2, C:NOR, NR4CO(R4)2, NR4SO2N(R4)2, NR4SO2R, or OCON(R4)2; R4 = R7, COR7, CO2(aliphatic), CON(R7)2, or SO2R7; or N(R4)2 = heterocyclyl or heteroaryl; R6 and R7 = independently H or (un) substituted aliphatic group; or N(R6)2 = heterocyclyl or heteroaryl; or N(R7)2 = heterocyclyl or heteroaryl; R9 = R, halo, OR, COR, CO2R, COCOR, etc.] were prepared as protein kinase inhibitors, especially

as

CN

inhibitors of Aurora-2 and GSK-3, for treating diseases such as cancer, diabetes, and Alzheimer's disease. Claims cover (pyrimidinyl)pyrazolamines and indazolamines I [wherein Z1 and Z2 = N; Z3 = CRx; Z4 = CRy; G = Ring C]. Examples include data for approx. 300 invention compds. prepared by a variety of synthetic methods and bioassay results for the inhibition of GSK- β 3, Aurora-2, ERK, and Src. For instance, the N-(4-pyrimidinyl)-3-pyrazolamine II was prepared and exhibited Ki values of < 0.1 μ M for glycogen synthetase kinase 3 β (GSK-3 β) and 0.1-1.0 μ M for Aurora-2.

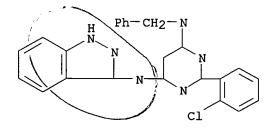
IT 404873-33-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(protein kinase inhibitor; preparation of heterocyclylpyrazolamines and analogs as protein kinase inhibitors for treatment of cancer, diabetes, and Alzheimer's disease)

RN 404873-33-2 CAPLUS

4,6-Pyrimidinediamine, 2-(2-chlorophenyl)-N-1H-indazol-3-yl-N'- (phenylmethyl)- (9CI) (CA INDEX NAME)



ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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     2002:220578 CAPLUS
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AB Triazolamines I and pyrazolamines II [wherein G = Ring C or Ring D; Ring C = (un)substituted Ph, pyridinyl, pyrimidinyl, pyridazinyl, pyrazinyl, or 1,2,4-triazinyl; Ring D = (un)substituted monocyclic or bicyclic ring selected from aryl, heteroaryl, heterocyclyl, or carbocyclyl; Z1 = N or CR9; Z2 = N or CH; Z3 = N or CRx; Z4 = N or CRy; Rx and Ry = independently

TR3, or taken together with their intervening atoms form an (un)saturated fused ring having 1-3 ring heteroatoms; R2 and R2a = independently R, TWR6; or C2R2R2a = (un) substituted fused ring containing 0-3 heteroatoms; T =a bond or alkylidene chain; W = C(R6)20, C(R6)2S0-2, C(R6)2NR6, CO, CO2, CR60CO, CR60CONR6, C(R6)2NR6CO, C(R6)2NR6CO2, CR6:NNR6, CR6:NO, C(R6) 2NR6NR6, C(R6) 2NR6SO2NR6, C(R6) 2NR6CONR6, or CONR6; R = H or (un) substituted aliphatic, (hetero) aryl, or heterocyclyl ring; R3 = R, halo, O, OR, COR, CO2R, COCOR, COCH2COR, NO2, CN, SO0-2R, N(R4)2, CON(R4)2, SO2N(R4)2, OCOR, NR4COR, NR4CO2(aliphatic), NR4N(R4)2, C:NN(R4)2, C:NOR, NR4CO(R4)2, NR4SO2N(R4)2, NR4SO2R, or OCON(R4)2; R4 = R7, COR7, CO2(aliphatic), CON(R7)2, or SO2R7; or N(R4)2 = heterocyclyl or heteroaryl; R6 and R7 = independently H or (un) substituted aliphatic group; or N(R6)2 = heterocyclyl or heteroaryl; or N(R7)2 = heterocyclyl or heteroaryl; R9 = R, halo, OR, COR, CO2R, COCOR, etc.] were prepared as protein kinase inhibitors, especially as inhibitors of Aurora-2 and GSK-3, for treating diseases such as cancer, diabetes, and Alzheimer's disease. Claims cover (heterocyclyl)triazolamines I [wherein Z1 = N or CR9; Z2 = N or CH; R9 is defined above]. Examples include data for approx. 300 invention compds. prepared by a variety of synthetic methods and bioassay results for the inhibition of GSK- β 3, Aurora-2, ERK, and Src. For instance, the N-(4-quinazolinyl)-1H-1,2,4-triazol-3-amine III was prepared and exhibited Ki values of $< 0.1 \mu M$ for glycogen synthetase kinase 3β (GSK-3 β) and 1.0-20 μ M for Aurora-2.

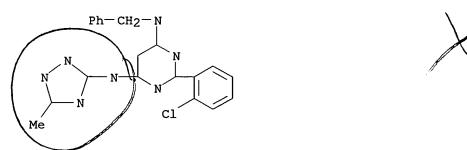
IT 404890-77-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(protein kinase inhibitor; preparation of triazolamines, pyrazolamines, and analogs as protein kinase inhibitors for treatment of cancer, diabetes, and Alzheimer's disease)

RN 404890-77-3 CAPLUS

CN 4,6-Pyrimidinediamine, 2-(2-chlorophenyl)-N-(5-methyl-1H-1,2,4-triazol-3-yl)-N'-(phenylmethyl)- (9CI) (CA INDEX NAME)



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AB
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     or (un) substituted (cyclo) alkyl, amino(alkoxy), or amidino; R6 = H, halo,
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     acyl(oxy), guanidinyl, (hetero)aryl, heterocyclo(alkyl), arylsulfonyl,
     arylsulfonamido, or (un) substituted alkyl, amino, etc.] were prepared as
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     alkylguanidine. The latter was cyclocondensed with resin-bound
     4-(MeCO)C6H4CONHCH2C6H4Br-3 and Cs2CO3 to afford, after resin cleavage,
     the pyrimidinamine II. The most preferred compds. of the invention
     exhibited inhibitory activity against human GSK3\beta in a cell free
     assay with IC50 values of < 1 \mu M. Thus, I and compns. containing I may be
     employed alone or in combination with other pharmacol. active agents in
     the treatment of disorders mediated by GSK3 activity, such as diabetes,
     Alzheimer's disease and other neurodegenerative disorders, obesity,
     atherosclerotic cardiovascular disease, essential hypertension, polycystic
```

ovary syndrome, syndrome X, ischemia, traumatic brain injury, bipolar disorder, immunodeficiency, or cancer (no data).

252904-40-8P, Benzonitrile, 4-[2-[[2-[(5-nitro-2-pyridinyl)amino]-4-pyrimidinyl]-

pyridinyl)amino[ethyl]amino]-5-[(phenylmethyl)amino]-4-pyrimidinyl]-RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

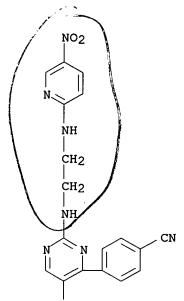
(preparation of aminopyrimidines and -pyridines as glycogen synthase kinase 3 inhibitors)

RN 252904-40-8 CAPLUS

ΙT

CN

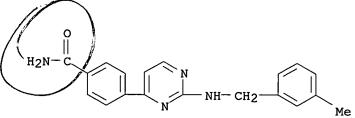
Benzonitrile, 4-[2-[[2-[(5-nitro-2-pyridinyl)amino]ethyl]amino]-5-[(phenylmethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)



Ph-CH2-NH

403806-74-6, 4-[2-[[(3-Methylphenyl)methyl]amino]pyrimidin-4-IT yl]benzamide 403806-75-7, 4-[2-[[(4-Aminophenyl)methyl]amino]pyrimidin-4-yl]benzamide 403806-80-4, 4-[2-[[(4-Cyanophenyl)methyl]amino]pyrimidin-4-yl]benzamide **403806-81-5**, 4-[2-[[(3-Methoxyphenyl)methyl]amino]pyrimidin-4yl]benzamide 403806-82-6, 4-[2-[[(4-Methoxyphenyl) methyl] amino] pyrimidin-4-yl] benzamide 403806-83-7, 4-[2-[[2-(4-Fluorophenyl)ethyl]amino]pyrimidin-4-yl]benzamide **403806-87-1**, 4-[2-[[(3-Chlorophenyl)methyl]amino]pyrimidin-4yl]benzamide 403806-92-8, 4-[2-[(4-Phenylbutyl)amino]pyrimidin-4yl]benzamide 403806-94-0, 4-[2-[[2-(3-Methoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzamide 403806-98-4, 4-[2-[[(3-Nitrophenyl)methyl]amino]pyrimidin-4-yl]benzamide 403807-02-3, 4-[2-[[2-(3-Chlorophenyl)ethyl]amino]pyrimidin-4yl]benzamide 403807-03-4, 4-[2-[(Naphthylmethyl)amino]pyrimidin-4-yl]benzamide 403807-07-8, 4-[2-[[2-(2,5-Dimethoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzenecarbonitrile 403807-11-4, 4-[2-[[2-(2H-Benzo[3,4-d]-1,3-dioxolan-5yl)ethyl]amino]pyrimidin-4-yl]benzamide 403807-12-5, 4-[2-[[2-(4-Nitrophenyl)ethyl]amino]pyrimidin-4-yl]benzamide 403807-13-6, 4-[2-[{(2,6-Dimethoxyphenyl)methyl}amino]pyrimidin-4yl]benzamide 403807-14-7, 4-[2-[[(3,4-

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Dimethoxyphenyl)methyl]amino]pyrimidin-4-yl]benzamide 403807-19-2
, 4-[2-[[[3-(Trifluoromethyl)phenyl]methyl]amino]pyrimidin-4-yl]benzamide
403807-20-5, 4-[2-[[[4-(Trifluoromethyl)phenyl]methyl]amino]pyrimi
din-4-yl]benzamide 403807-21-6, 4-[2-[[(3,5-
Dichlorophenyl)methyl]amino]pyrimidin-4-yl]benzamide 403807-23-8
, 4-[2-[(2,4-Dichlorophenyl)methyl]amino]pyrimidin-4-yl]benzamide
403807-37-4, 4-[2-[(4-Bromophenyl)methyl]amino]pyrimidin-4-
yl]benzamide 403807-38-5, 4-[2-[[[4-(4-
Fluorophenyl)phenyl]methyl]amino]pyrimidin-4-yl]benzamide
403807-39-6, 4-[2-[[(3-Bromophenyl)methyl]amino]pyrimidin-4-
yl]benzamide 403807-47-6, 4-[2-[[(3,4,5-
Trimethoxyphenyl)methyl]amino]pyrimidin-4-yl]benzamide 403807-49-8
, 4-[2-[[[3-(3-Aminophenyl)phenyl]methyl]amino]pyrimidin-4-yl]benzamide
403807-50-1, 4-[2-[[[4-(3-Aminophenyl)phenyl]methyl]amino]pyrimidi
n-4-yl]benzamide 403807-53-4, Ethyl 4-(4-cyanophenyl)-2-[[2-(3-
methoxyphenyl)ethyl]amino]pyrimidine-5-carboxylate 403807-60-3,
4-[2-[[[3-(3-Methoxyphenyl)phenyl]methyl]amino]pyrimidin-4-yl]benzamide
403807-65-8, 4-[2-[[[3-[3-[(Methylamino)methyl]phenyl]phenyl]methy
l]amino]pyrimidin-4-yl]benzamide 403807-78-3,
4-[2-[[[3-[3-(Acetylamino)phenyl]phenyl]methyl]amino]pyrimidin-4-
yl]benzamide 403807-79-4, 4-[2-[[[3,5-
Bis(trifluoromethyl)phenyl]methyl]amino]pyrimidin-4-yl]benzamide
403807-83-0, 4-[2-[[[3-[3-(Trifluoromethyl)phenyl]phenyl]methyl]am
ino]pyrimidin-4-yl]benzamide 403808-16-2, [4-[2-[[(3-
Bromophenyl)methyl]amino]pyrimidin-4-yl]phenyl]-N-[(3-
methylphenyl) methyl] carboxamide 403808-32-2,
N-[(3-Bromophenyl)methyl]-4-[2-[[2-(3-methoxyphenyl)ethyl]amino]pyrimidin-
4-yl]phenylcarboxamide 403808-46-8 403809-22-3,
4-[2-[[2-(2,5-Dimethoxyphenyl)ethyl]amino]pyrimidin-4-yl]benzamide
403809-23-4, 4-[2-[[2-(2,3-Dimethoxyphenyl)ethyl]amino]pyrimidin-4-
yl]benzamide 403810-50-4
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
   (preparation of aminopyrimidines and -pyridines as glycogen synthase kinase
   3 inhibitors)
403806-74-6 CAPLUS
Benzamide, 4-[2-[[(3-methylphenyl)methyl]amino]-4-pyrimidinyl]- (9CI)
                                                                        (CA
INDEX NAME)
```



RN 403806-75-7 CAPLUS

RN

CN

CN Benzamide, 4-[2-[[(4-aminophenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \circ \\ \vdots \\ \text{H}_2\text{N}-\text{C} \\ \hline \\ N \end{array} \qquad \text{NH-CH}_2$$

RN 403806-80-4 CAPLUS

CN Benzamide, 4-[2-[[(4-cyanophenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} C & & C \\ H_2N-C & & N \\ \hline & NH-CH_2 \\ \hline \end{array}$$

RN 403806-81-5 CAPLUS

CN Benzamide, 4-[2-[[(3-methoxyphenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 403806-82-6 CAPLUS

CN Benzamide, 4-[2-[[(4-methoxyphenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O \\ \parallel \\ H_2N-C \\ \hline \\ N \\ \hline \\ N \\ NH-CH_2 \\ \hline \end{array} \begin{array}{c} OMe \\ \end{array}$$

RN 403806-83-7 CAPLUS

CN Benzamide, 4-[2-[[2-(4-fluorophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$H_2N-C$$
 N
 $NH-CH_2-CH_2$

RN 403806-87-1 CAPLUS

CN Benzamide, 4-[2-[[(3-chlorophenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} O \\ H_2N-C \\ \hline \\ N \\ \end{array}$$

$$NH-CH_2$$

RN 403806-92-8 CAPLUS

CN Benzamide, 4-[2-[(4-phenylbutyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 403806-94-0 CAPLUS

CN Benzamide, 4-[2-[[2-(3-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \circ & \\ H_2N-C & & N \\ \hline & N & NH-CH_2-CH_2 \\ \hline & OMe \\ \end{array}$$

RN 403806-98-4 CAPLUS

CN Benzamide, 4-[2-[[(3-nitrophenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \circ \\ \parallel \\ \text{H}_2\text{N}-\text{C} \\ \hline \\ \end{array} \\ \begin{array}{c} \text{N} \\ \text{NH}-\text{CH}_2 \\ \hline \\ \end{array} \\ \begin{array}{c} \text{NO}_2 \\ \end{array}$$

RN 403807-02-3 CAPLUS

CN Benzamide, 4-[2-[[2-(3-chlorophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \circ \\ \text{H}_2\text{N}-\text{C} \\ \hline \\ \text{N} \\ \end{array} \\ \text{NH-CH}_2-\text{CH}_2 \\ \end{array}$$

RN 403807-03-4 CAPLUS

CN Benzamide, 4-[2-[(1-naphthalenylmethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 403807-07-8 CAPLUS

CN Benzonitrile, 4-[2-[[2-(2,5-dimethoxyphenyl)ethyl]amino]-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{OMe} \\ \hline \\ \text{NC} & \text{NH-} \text{CH}_2\text{--} \text{CH}_2 \\ \hline \\ \text{OMe} \\ \end{array}$$

RN 403807-11-4 CAPLUS

CN Benzamide, 4-[2-[[2-(1,3-benzodioxol-5-yl)ethyl]amino]-4-pyrimidinyl]-

(9CI) (CA INDEX NAME)

$$\begin{array}{c} \circ \\ H_2N-C \\ \hline \\ N \\ \end{array} \\ NH-CH_2-CH_2 \\ \hline \\ O \\ \end{array}$$

RN 403807-12-5 CAPLUS

CN Benzamide, 4-[2-[[2-(4-nitrophenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ H_2N-C & & & \\ \hline & N & NH-CH_2-CH_2 \\ \hline \end{array}$$

RN 403807-13-6 CAPLUS

CN Benzamide, 4-[2-[[(2,6-dimethoxyphenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ H_2N-C & \\ \hline & N \\ \hline & NH-CH_2 \\ \hline & OMe \\ \end{array}$$

RN 403807-14-7 CAPLUS

CN Benzamide, 4-[2-[[(3,4-dimethoxyphenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & OMe \\ H_2N-C & N & NH-CH_2 \\ \hline \end{array}$$

RN 403807-19-2 CAPLUS

CN Benzamide, 4-[2-[[[3-(trifluoromethyl)phenyl]methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$H_2N-C$$
 N
 $NH-CH_2$
 CF_3

RN 403807-20-5 CAPLUS

CN Benzamide, 4-[2-[[[4-(trifluoromethyl)phenyl]methyl]amino]-4-pyrimidinyl]-(9CI) (CA INDEX NAME)

$$H_2N-C$$
 N
 $N+CH_2$
 CF_3

RN 403807-21-6 CAPLUS

CN Benzamide, 4-[2-[[(3,5-dichlorophenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & C1 \\ H_2N-C & N \\ \hline & N \\ & N+CH_2 \\ \hline & C \\ \end{array}$$

RN 403807-23-8 CAPLUS

CN Benzamide, 4-[2-[[(2,4-dichlorophenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$H_2N-C$$
 N
 $NH-CH_2$
 $C1$

RN 403807-37-4 CAPLUS

CN Benzamide, 4-[2-[[(4-bromophenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 403807-38-5 CAPLUS

CN Benzamide, 4-[2-[[(4'-fluoro[1,1'-biphenyl]-4-yl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & & & \\ H_2N-C & & & \\ \hline & N & NH-CH_2 \end{array}$$

RN 403807-39-6 CAPLUS

CN Benzamide, 4-[2-[[(3-bromophenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$H_2N-C$$
 N
 $NH-CH_2$
 B_1

RN 403807-47-6 CAPLUS

CN Benzamide, 4-[2-[[(3,4,5-trimethoxyphenyl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & \\ \text{M} & \text{NH-CH}_2 \\ & & \\ \text{OMe} \\ \end{array}$$

RN 403807-49-8 CAPLUS

CN Benzamide, 4-[2-[[(3'-amino[1,1'-biphenyl]-3-yl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O \\ H_2N-C \\ \hline \\ N \\ NH-CH_2 \\ \hline \\ NH_2 \\ \end{array}$$

RN 403807-50-1 CAPLUS

CN Benzamide, 4-[2-[[(3'-amino[1,1'-biphenyl]-4-yl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \circ & & \\ H_2N-C & & & \\ \hline & N & NH-CH_2 & & \\ \hline \end{array}$$

RN 403807-53-4 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-(4-cyanophenyl)-2-[[2-(3-methoxyphenyl)ethyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 403807-60-3 CAPLUS

CN Benzamide, 4-[2-[[(3'-methoxy[1,1'-biphenyl]-3-yl)methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 403807-65-8 CAPLUS

CN Benzamide, 4-[2-[[[3'-[(methylamino)methyl][1,1'-biphenyl]-3-yl]methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O \\ C-NH_2 \end{array}$$

$$MeNH-CH_2$$

RN 403807-78-3 CAPLUS

CN Benzamide, 4-[2-[[[3'-(acetylamino)[1,1'-biphenyl]-3-yl]methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O \\ \parallel \\ C-NH_2 \end{array}$$

RN 403807-79-4 CAPLUS

CN Benzamide, 4-[2-[[[3,5-bis(trifluoromethyl)phenyl]methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 403807-83-0 CAPLUS

CN Benzamide, 4-[2-[[[3'-(trifluoromethyl)[1,1'-biphenyl]-3-yl]methyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$c-NH_2$$

RN 403808-16-2 CAPLUS

CN Benzamide, 4-[2-[[(3-bromophenyl)methyl]amino]-4-pyrimidinyl]-N-[(3-methylphenyl)methyl]- (9CI) (CA INDEX NAME)

$$Br$$
 CH_2-NH N $C-NH-CH_2$

RN 403808-32-2 CAPLUS

CN Benzamide, N-[(3-bromophenyl)methyl]-4-[2-[[2-(3-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

MeO
$$CH_2-CH_2-NH$$
 N $C-NH-CH_2$

RN 403808-46-8 CAPLUS

CN Benzamide, N-[(3-bromophenyl)methyl]-4-[2-[[2-(2,5-dimethoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 403809-22-3 CAPLUS

CN Benzamide, 4-[2-[[2-(2,5-dimethoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \mathsf{O} & \mathsf{OMe} \\ \mathsf{H}_2\mathsf{N}-\mathsf{C} & \mathsf{N} \\ \mathsf{N} & \mathsf{NH}-\mathsf{CH}_2-\mathsf{CH}_2 \\ \hline \\ \mathsf{OMe} \end{array}$$

RN 403809-23-4 CAPLUS

CN Benzamide, 4-[2-[[2-(2,3-dimethoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$H_2N-C$$
 N
 N
 $N+CH_2-CH_2$

OMe

RN 403810-50-4 CAPLUS

CN Benzamide, 4-[2-[[2-(2-methoxyphenyl)ethyl]amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{O} \\ \text{H}_2\text{N}-\text{C} \\ \\ \text{N} \end{array} \qquad \text{NH-CH}_2-\text{CH}_2 \\ \end{array}$$

```
ANSWER 67 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
L10
AN
     2002:171866 CAPLUS
     136:232313
DN
     Preparation of pyrimidine derivatives as G protein-coupled receptor kinase
TΙ
     (GRK) inhibitors
     Fukumoto, Shoji; Watanabe, Toshifumi; Ikeda, Shota
IN
PA
     Takeda Chemical Industries, Ltd., Japan
SO
     PCT Int. Appl., 322 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     Japanese
FAN.CNT 1
     PATENT NO.
                          KIND
                                  DATE
                                              APPLICATION NO.
                                                                         DATE
                           ----
                                   _____
                                               ______
                                   20020307
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                                                                         20010829
PΙ
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              GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS,
             LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT,
              RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US,
         RO, RO, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                  20020313
                                             AU 2001-82520
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     AU 2001082520
                            A5
                                   20020522
                                                JP 2001-259683
                                                                         20010829
     JP 2002145778
                            A2
PRAI JP 2000-264499
                                   20000829
                            Α
     WO 2001-JP7397
                                   20010829
os
     MARPAT 136:232313
AB
     Disclosed are novel GRK inhibitors which contains compds. represented by
     the formula (I), a salt thereof, or a prodrug comprising either of these
     (wherein ring A represents optionally further substituted nitrogen-containing
     heterocycle; R1 and R2 each represents optionally substituted amino; and X
     represents a spacer comprising a linear part constituted of one to four
     atoms, provided that R1 may be bonded to R2 or/and X to form a ring).
     They are useful as preventives/remedies for cardiac failure. Thus, 5.48 g
     K2CO3 and 7.52 g 2-aminophenyl 2-nitrophenyl sulfide were added to a
     suspension of 5.61 g 4-amino-5-bromomethyl-2-methylpyrimidine hydrobromide
     in 40 mL acetone at room temperature and stirred at 65° for 64 h to give
     2.36 g N-[(4-amino-2-methyl-5-pyrimidinyl)methyl]-N-[2-[(2-
     nitrophenyl)thio]phenyl]amine (II). All 10 compds. tested including II at
     30 µM inhibited 30% human GRK2 expressed by human GRK2 gene in COS-7
     cells. A capsule and a tablet formulation containing II were also prepared
IT
     403514-78-3P 403514-79-4P 403516-08-5P
     403516-29-0P 403516-31-4P 403516-36-9P
     403516-40-5P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
         (preparation of pyrimidine derivs. as G protein-coupled receptor kinase
        (GRK) inhibitors for prevention and/or treatment for cardiac failure)
RN
     403514-78-3 CAPLUS
     Benzoic acid, 2-[[(4-amino-2-phenyl-5-pyrimidinyl)methyl]amino]-,
```

Double bond geometry as shown.

(2E)-3-phenyl-2-propenyl ester (9CI) (CA INDEX NAME)

RN 403514-79-4 CAPLUS

CN Formamide, N-[(4-amino-2-phenyl-5-pyrimidinyl)methyl]-N-[2-[(2-ethoxyethyl)thio]phenyl]- (9CI) (CA INDEX NAME)

RN 403516-08-5 CAPLUS

CN Formamide, N-[(4-amino-2-phenyl-5-pyrimidinyl)methyl]-N-[2-[[[(phenylmethyl)thio]methyl]thio]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ \text{Ph-CH}_2-\text{S-CH}_2-\text{S} & & & \\ \end{array}$$

RN 403516-29-0 CAPLUS

CN 5-Pyrimidinemethanamine, 4-amino-N-[2-[(4-methoxyphenyl)thio]phenyl]-2-phenyl- (9CI) (CA INDEX NAME)

RN 403516-31-4 CAPLUS

CN Formamide, N-[(4-amino-2-phenyl-5-pyrimidinyl)methyl]-N-[2-[(4-methoxyphenyl)thio]phenyl]- (9CI) (CA INDEX NAME)

RN 403516-36-9 CAPLUS

CN 5-Pyrimidinemethanamine, 4-amino-N-[2-[(2-nitrophenyl)thio]phenyl]-2-phenyl- (9CI) (CA INDEX NAME)

RN 403516-40-5 CAPLUS

CN Formamide, N-[(4-amino-2-phenyl-5-pyrimidinyl)methyl]-N-[2-[(2-nitrophenyl)thio]phenyl]- (9CI) (CA INDEX NAME)

```
ANSWER 68 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
L10
AN
     2002:122770 CAPLUS
DN
     136:178015
     Drugs for incontinence - salified and nonsalified nitric oxide-donors and
TI
     phosphodiesterase inhibitors
     Del Soldato, Piero; Benedini, Francesca
IN
PA
     Nicox S.A., Fr.
     PCT Int. Appl., 59 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LА
     English
FAN.CNT 1
                                                                    DATE
                                            APPLICATION NO.
                         KIND
                                DATE
     PATENT NO.
                                            ______
                                            WO 2001-EP8734
                                                                    20010727
     WO 2002011707
                          A2
                                20020214
PΙ
                                20021205
     WO 2002011707
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             LV, MA, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA,
             US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                                20030827
                                            IT 2000-MI1848
                                                                    20000808
     IT 1318674
                          В1
                                            AU 2001-91691
                                                                    20010727
     AU 2001091691
                          A5
                                20020218
                                                                    20010727
                                            EP 2001-971798
                                20030507
     EP 1307184
                          A2
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
                                             JP 2002-517044
                                                                    20010727
     JP 2004511436
                          T2
                                20040415
                                            US 2003-343330
                                                                    20030206
                                20031030
     US 2003203899
                          A1
                                20000808
PRAI IT 2000-MI1848
                          Α
     WO 2001-EP8734
                          W
                                20010727
     MARPAT 136:178015
OS
     Use in the incontinence of one or more of the following classes of drugs
AB
     selected from the following: (B) salified and nonsalified nitric
     oxide-donor drugs, of formula: A - X1 - N(O)z, (B') nitrate salts of drugs
     used for the incontinence, and which do not contain in the mol. a nitric
     oxide donor group; (C) organic or inorg. salts of compds. inhibiting
     phosphodiesterases.
ΙT
     398454-66-5
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (salified and nonsalified nitric oxide-donors and phosphodiesterase
        inhibitors for treatment of incontinence)
RN
     398454-66-5 CAPLUS
     4-Pyrimidinamine, N-(1,3-benzodioxol-5-ylmethyl)-2-(1H-imidazol-1-yl)-5-
CN
     phenyl- (9CI)
                   (CA INDEX NAME)
                   -CH2
```

```
ANSWER 69 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
L10
     2002:122769 CAPLUS
AN
     136:189342
DN
     Drugs for treatment of sexual dysfunction
TI
IN
     Del Soldato, Piero
     Nicox S.A., Fr.
PA
     PCT Int. Appl., 40 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
                                  DATE
                                              APPLICATION NO.
                                                                        DATE
     PATENT NO.
                          KIND
                                               _____
                          ____
                                  _____
                                               WO 2001-EP8733
                                                                        20010727
                           A2
                                  20020214
PΙ
     WO 2002011706
     WO 2002011706
                           А3
                                  20030918
         W: AE, AG, AL, AU, BA, BB, BG, BR, BZ, CA, CN, CR, CU, CZ, DM, DZ,
             EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA,
             US, UZ, VN, YU, ZA
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR,
             IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN,
             GQ, GW, ML, MR, NE, SN, TD, TG
                                                                        20000808
     IT 1318673
                           В1
                                  20030827
                                               IT 2000-MI1847
     AU 2001091690
                           A5
                                  20020218
                                               AU 2001-91690
                                                                        20010727
                                  20031126
                                               EP 2001-971797
                                                                        20010727
     EP 1363628
                           A2
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, SI, LT, FI, RO, CY, TR
                                               JP 2002-517043
                                                                        20010727
                                  20040304
     JP 2004506619
                           Т2
                           Α1
                                  20030911
                                               US 2003-333927
                                                                        20030204
     US 2003171393
PRAI IT 2000-MI1847
                           Α
                                  20000808
     WO 2001-EP8733
                           W
                                  20010727
     MARPAT 136:189342
     Pharmaceuticals containing nitric oxide-donor drugs or inorg. salts of compds.
AΒ
     inhibiting phosphodiesterases are useful for the treatment of sexual
     dysfunction. Thus, a formulation contained 2-(acetyloxy)benzoic acid
     6-(nitroxy-methyl)-2-methylpyridyl ester-HCl (NCX 4050) 4.2, white
     petrolatum 24, Polysorbate-60 4.8, glycerin 9.5, and water 48 g. NCX 4050
     showed vasorelaxing activity on the aortas.
IT
     398460-38-3
     RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
         (drugs for treatment of sexual dysfunction)
     398460-38-3 CAPLUS
RN
     4-Pyrimidinamine, N-(1,3-benzodioxol-5-ylmethyl)-2-(1H-imidazol-1-yl)-5-
CN
     phenyl-, nitrate (9CI) (CA INDEX NAME)
     CM
     CRN
          398454-66-5
     CMF C21 H17 N5 O2
                NH-CH2
```

CM 2

CRN 7697-37-2 CMF H N O3



10/671,070

L10 ANSWER 70 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 2002:96165 CAPLUS

DN 136:294745

TI A Combinatorial Scaffold Approach toward Kinase-Directed Heterocycle Libraries

AU Ding, Sheng; Gray, Nathanael S.; Wu, Xu; Ding, Qiang; Schultz, Peter G.

CS Department of Chemistry and the Skaggs Institute for Chemical Biology, The Scripps Research Institute, La Jolla, CA, 92037, USA

SO Journal of the American Chemical Society (2002), 124(8), 1594-1596 CODEN: JACSAT; ISSN: 0002-7863

PB American Chemical Society

DT Journal

LA English

OS CASREACT 136:294745

AB A novel strategy for efficient synthesis of various substituted nitrogen-heterocycles, e.g., I, as kinase-directed combinatorial libraries is described. The general scheme involves capture of various dichloroheterocycles onto solid support and further elaborations by aromatic substitution with amines at elevated temperature or by anilines, boronic acids, and phenols via palladium-catalyzed cross-coupling reactions, thus the scaffold itself is transformed into a diversity element within the combinatorial scheme. Libraries consisting of discrete and highly diverse heterocyclic small mols. constructed with these chemistries are currently being evaluated in a variety of cell and protein-based assays.

IT 406932-41-0P 406932-42-1P 406932-43-2P

406932-44-3P 406932-45-4P

RL: CPN (Combinatorial preparation); CMBI (Combinatorial study); PREP (Preparation)

(derivatization of resin bound chloroheterocyclic scaffolds via Suzuki coupling reaction with aryl boronic acid and subsequent cleavage of substituted heterocyclic product)

RN 406932-41-0 CAPLUS

CN 4-Pyrimidinamine, 2-(3-methoxyphenyl)-N-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)

RN 406932-42-1 CAPLUS

CN 4-Pyrimidinamine, 2-(3-methoxyphenyl)-N-[(4-methoxyphenyl)methyl]-5-methyl-(9CI) (CA INDEX NAME)

RN 406932-43-2 CAPLUS

CN 4-Pyrimidinamine, 2-(3-methoxyphenyl)-N-[(4-methoxyphenyl)methyl]-6-methyl-(9CI) (CA INDEX NAME)

RN 406932-44-3 CAPLUS

CN 4-Pyrimidinamine, 6-(3-methoxyphenyl)-N-[(4-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)

RN 406932-45-4 CAPLUS

CN 2,4-Pyrimidinediamine, 6-(3-methoxyphenyl)-N4-[(4-methoxyphenyl)methyl](9CI) (CA INDEX NAME)

RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/671,070

- L10 ANSWER 71 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2002:54948 CAPLUS
- DN 136:363251
- TI Bioisosterism, enantioselectivity, and molecular modeling of new effective N6- and/or N(9)-substituted 2-phenyladenines and 8-aza analogs: different binding modes to Al adenosine receptors
- AU Bianucci, A. Maria; Biagi, Giuliana; Coi, Alessio; Giorgi, Irene; Oreste, Livi; Pacchini, Federica; Scartoni, Valerio; Lucacchini, Antonio; Costa, Barbara
- CS Department of Pharmaceutical Sciences, University of Pisa, Pisa, 56126, Italy
- SO Drug Development Research (2001), 54(2), 52-65 CODEN: DDREDK; ISSN: 0272-4391
- PB Wiley-Liss, Inc.
- DT Journal
- LA English
- OS CASREACT 136:363251
- Bioisosterism of the adenine and 8-azaadenine nuclei was demonstrated by comparison of Al adenosine receptor binding affinity of 2-Ph N6-substituted adenines and the corresponding 8-azaadenines. Some of these new compds. are very potent Al adenosine receptor antagonists. This work also describes the synthesis and Al adenosine receptor binding of the enantiomers of some 2-phenyladenines substituted with a 1-phenylethyl chiral group in N6 and N(9) positions. Biol. results, showing the same stereoselectivity for all the couples of enantiomers, may supply proof for the hypothesis of a possible double arrangement of 2-phenylsubstituted adenines inside Al adenosine receptors. Theor. studies, based on an improved Al adenosine receptor model and consisting of evaluation and comparison of interaction energies in complexes involving some selected chiral ligands, support the above hypothesis.
- IT 424830-65-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(bioisosterism, enantioselectivity, and mol. modeling of new effective phenyladenines and aza analogs and different binding modes to Al adenosine receptors)

- RN 424830-65-9 CAPLUS
- CN 4,5-Pyrimidinediamine, 6-chloro-2-phenyl-N4-(phenylmethyl)- (9CI) (CA INDEX NAME)

RE.CNT 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 72 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
L10
AN
     2001:816647 CAPLUS
     135:357948
DN
     Preparation of heterocyclic compounds as phosphodiesterase V (PDE V)
TI
     inhibitors
     Yamada, Koichiro; Matsuki, Kenji; Omori, Kenji; Kikkawa, Kohei
IN
PA
     Tanabe Seiyaku Co., Ltd., Japan
SO
     PCT Int. Appl., 207 pp.
     CODEN: PIXXD2
DT
     Patent
     Japanese
LΑ
FAN.CNT 3
                                             APPLICATION NO.
                                                                     DATE
                         KIND
                                 DATE
     PATENT NO.
                          ____
                                             WO 2001-JP2034
                                                                     20010315
ΡI
     WO 2001083460
                          A1
                                 20011108
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM,
             HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT,
             LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
             SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
             YU, ZA, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     AU 2001041142
                                             AU 2001-41142
                          A5
                                 20011112
                                                                     20010315
     CA 2407231
                          AΑ
                                 20021023
                                             CA 2001-2407231
                                                                     20010315
     EP 1277741
                          A1
                                 20030122
                                             EP 2001-912373
                                                                     20010315
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
                                             NZ 2001-522217
     NZ 522217
                          Α
                                 20040430
                                                                     20010315
                                             CN 2004-10098098
                                 20050824
                                                                     20010315
     CN 1657523
                          Α
                                 20031211
                                             US 2002-258545
                                                                     20021025
     US 2003229089
                          Α1
                                             US 2003-699804
                                                                     20031104
                                 20040722
     US 2004142930
                          Α1
                                             AU 2005-203687
                                                                     20050817
                                 20050908
     AU 2005203687
                          A1
PRAI JP 2000-130371
                          Α
                                 20000428
     JP 2000-277652
                          Α
                                 20000913
     AU 2001-41142
                          А3
                                 20010315
     WO 2001-JP2034
                                 20010315
     US 2002-258545
                                 20021025
                          A2
OS
     MARPAT 135:357948
     Compds. of the general formula (I) or pharmacol. acceptable salts thereof
AB
     [wherein X is :CH or N; Y is NH, NR4, S, O, CH:N, N:CH, N:N, CH:CH, or the
     like; R1 is lower alkoxy, amino, a nitrogenous heterocyclic group, or a
     hydroxyl group substituted with a heterocyclic group (wherein each group
     may be substituted); R2 is either a lower alkylamino or lower alkoxy group
     which may be substituted with aryl, or a lower alkoxy group substituted
     with a nitrogenous aromatic heterocyclic group; and R3 is aryl, a nitrogenous
     heterocyclic group, lower alkyl, lower alkoxy, lower cycloalkoxy, a
     hydroxyl group substituted with a nitrogenous heterocyclic group, or amino
     (wherein each group may be substituted), or alternatively, R3 and the
     substituent of Y may be united to form a lactone ring] or pharmacol.
     acceptable salts thereof are prepared These compds. exhibit excellent PDE V
     inhibitory activity and are useful as preventive or therapeutic agents for
     various diseases due to dysfunction of the signal transduction through
     cGMP, in particular impotence, pulmonary hypertension, and diabetic renal
     failure paralysis (no data). Thus, 2-(hydroxymethyl)pyridine was treated
     wit NaH in THF at room temperature for 30 min and then condensed with
```

2-chloro-5-(3,4,5-trimethoxyphenylcarbonyl)-4-(3-chloro-4-

 $\label{eq:methoxybenzylamino} \mbox{pyrimidine (preparation given) in THF at room temperature} \\ \mbox{for } 1 \ \mbox{h}$

to give 2-(2-pyridylmethoxy)-5-(3,4,5-trimethoxyphenylcarbonyl)-4-(3-chloro-4-methoxybenzylamino)pyrimidine.

IT 372117-36-7P 372117-37-8P 372117-38-9P 372117-39-0P 372117-40-3P 372117-41-4P 372117-44-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heterocyclic compds. as phosphodiesterase V inhibitors preventive or therapeutic agents for various diseases due to dysfunction of signal transduction through cGMP)

RN 372117-36-7 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[(3-chloro-4-methoxyphenyl)methyl]amino]-2-(2-pyridinylmethoxy)-6-(3,4,5-trimethoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 372117-37-8 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[(3-chloro-4-methoxyphenyl)methyl]amino]-2-(4-hydroxy-1-piperidinyl)-6-(3,4,5-trimethoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)

Page 564

RN 372117-38-9 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[(3-chloro-4-methoxyphenyl)methyl]amino]-2[2-(hydroxymethyl)-4-morpholinyl]-6-(3,4,5-trimethoxyphenyl)-, methyl
ester (9CI) (CA INDEX NAME)

RN 372117-39-0 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[(3-chloro-4-methoxyphenyl)methyl]amino]-2[(2-methoxyethyl)methylamino]-6-(3,4,5-trimethoxyphenyl)-, methyl ester
(9CI) (CA INDEX NAME)

RN 372117-40-3 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[(3-chloro-4-methoxyphenyl)methyl]amino]-2[2-(dimethylamino)ethoxy]-6-(3,4,5-trimethoxyphenyl)-, methyl ester (9CI)
(CA INDEX NAME)

RN 372117-41-4 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[(3-chloro-4-methoxyphenyl)methyl]amino]-2-(1-piperazinyl)-6-(3,4,5-trimethoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & H \\ N \\ \hline \\ N \\ \hline \\ CH_2-NH \\ \hline \\ C-OMe \\ \hline \\ O \\ \end{array} \\ \begin{array}{c} OMe \\ OMe \\ \hline \\ OMe \\ \end{array}$$

RN 372117-44-7 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 2-[bis(2-hydroxyethyl)amino]-4-[[(3-chloro-4-methoxyphenyl)methyl]amino]-6-(3,4,5-trimethoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 73 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
L10
     2001:635876 CAPLUS
ΑN
     135:211049
DN
     Preparation of pyrimidinamines and pyridinamines as adenosine receptor
ΤI
     modulators for treatment of CNS disorders
     Borroni, Edilio Maurizio; Huber-Trottmann, Gerda; Kilpatrick, Gavin John;
IN
     Norcross, Roger David
     F. Hoffmann La Roche A.-G., Switz.
PA
     PCT Int. Appl., 256 pp.
SO
     CODEN: PIXXD2
DΤ
     Patent
     English
LΑ
FAN.CNT 1
                                                                    DATE
                                            APPLICATION NO.
                         KIND
                                DATE
     PATENT NO.
                                            _____
                         ____
                                            WO 2001-EP1679
                                                                    20010215
                          A2
                                20010830
     WO 2001062233
PΙ
                          A3
                                20020103
     WO 2001062233
             AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ,
             DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS,
             JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG,
             MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL,
             TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                                                    20010215
                                             CA 2001-2398274
     CA 2398274
                          AΑ
                                20010830
                                                                    20010215
                                             EP 2001-927670
                          A2
                                 20021204
     EP 1261327
                                 20050427
     EP 1261327
                          В1
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
                                 20030506
                                             BR 2001-8611
                                                                    20010215
     BR 2001008611
                          Α
                                                                    20010215
                                 20030805
                                             JP 2001-561300
     JP 2003523380
                          T2
                                                                    20010215
                                             NZ 2001-520241
                                 20040528
     NZ 520241
                          Α
                                             AU 2001-54643
                                                                    20010215
                                 20050324
     AU 780527
                          В2
                                             AT 2001-927670
                                                                    20010215
                                 20050515
     AT 293962
                          Ε
                                                                    20010215
                                             ES 2001-1927670
                                 20051016
                          Т3
     ES 2240449
                                             US 2001-788956
                                                                    20010220
                                 20011004
     US 2001027196
                          A1
                                 20030701
     US 6586441
                          В2
                                                                    20020730
                                             ZA 2002-6077
                                 20031030
     ZA 2002006077
                          Α
                                             NO 2002-4006
                                                                    20020822
     NO 2002004006
                          Α
                                 20020822
PRAI EP 2000-103432
                          Α
                                 20000225
     WO 2001-EP1679
                           W
                                 20010215
     MARPAT 135:211049
OS
     The title compds. (I) [wherein A = a bond, S, N(R), (CH2)2, CH:CH,
AB
     C.tplbond.C, or O; X and Y = independently N:, :N, :CH, C(CN):, :C(CN),
     C(CSNH2):, or :C(CSNH2), wherein at least 1 of X or Y is N; R1 = H,
      (cyclo)alkyl, alkenyl, alkynyl, halo, CN, (alkyl)carboxylates,
      (alkyl)carbamates, alkoxy(alkyl), phenoxy(alkyl), phenylamino(alkyl),
      (un) substituted phenyl(alkyl) or amino(alkyl), morpholinyl(alkyl),
     piperidinyl(alkyl), pyridinyl(alkyl), piperazinyl(alkyl), etc.; R2 = H,
     halo, CN, NO2, acyl, carboxylate, (un) substituted alkyl, alkenyl, alkynyl,
     or Ph; R3 = alkyl or thienyl, (dihydro)furanyl, benzodioxolyl, isoxazolyl,
     pyridinyl, dihydropyranyl, pyrazinyl, aryl(alkyl)oxy, pyrazolyl,
      (un) substituted Ph, etc.; R4 and R5 = independently H, benzoyl, or
      (un) substituted phenacyl; or A and R2 taken together the with the C atoms
     to which they are attached may form a substituted thienyl group] were
     prepared as adenosine receptor modulators. For example, treating
      3,4,5-trimethoxybenzoylacetonitrile with to NaH in DMSO, followed by addition
```

of CS2 and MeI, gave the bis(methylthio) intermediate. Cycloaddn. with guanidine nitrate in the presence of TEA in DMF afforded the pyrimidinenitrile (II), which exhibited high selectivity toward the A1 and A3 adenosine receptors compared to the A2 receptor with pKi values of 5.88, 5.71 and 7.24, resp. I are useful for the treatment of Alzheimer's disease, Parkinson's disease, neuroprotection, schizophrenia, anxiety, pain, respiration deficits, depression, asthma, allergic responses, hypoxia, ischemia, seizure, substance abuse, and sedation, and they may be active as muscle relaxants, antipsychotics, antiepileptics, anticonvulsants, and cardioprotective agents (no data). The most preferred indications for I are those which include disorders of the central nervous system, such as certain depressive disorders, neuroprotection, and Parkinson's disease.

IT 357285-14-4P 357285-22-4P 357285-25-7P 357285-37-1P 357288-80-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrimidinamines and pyridinamines as adenosine receptor modulators for treatment of CNS disorders and other diseases)

RN 357285-14-4 CAPLUS

5-Pyrimidinecarbonitrile, 2-amino-4-phenyl-6-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 357285-22-4 CAPLUS

CN 5-Pyrimidinecarbonitrile, 2-amino-4-phenyl-6-[(3-phenylpropyl)amino](9CI) (CA INDEX NAME)

RN 357285-25-7 CAPLUS

CN 5-Pyrimidinecarbonitrile, 2-amino-4-phenyl-6-[(2-phenylethyl)amino]- (9CI) (CA INDEX NAME)

RN 357285-37-1 CAPLUS

CN 5-Pyrimidinecarbonitrile, 2-amino-4-[[2-(4-hydroxyphenyl)ethyl]amino]-6-phenyl- (9CI) (CA INDEX NAME)

RN 357288-80-3 CAPLUS

CN 5-Pyrimidinecarbonitrile, 2-amino-4-(2-methoxyphenyl)-6-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{NH}_2 \\ & \text{N} \\ & \text{N} \\ & \text{N} \\ & \text{CN} \\ \end{array}$$

```
ANSWER 74 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
     2001:597969 CAPLUS
AN
     135:180777
DN
ΤI
     Preparation of 2-pyrimidinamines as selective inhibitors of COX-2
IN
     Carter, Malcolm Clive; Naylor, Alan; Payne, Jeremy John; Pegg, Neil
     Glaxo Group Ltd., UK
PA
     PCT Int. Appl., 38 pp.
SO
     CODEN: PIXXD2
DΤ
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                    DATE
PΙ
     WO 2001058881
                          A1
                                20010816
                                            WO 2001-GB511
                                                                    20010208
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN
             CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
             HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
             LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,
             SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
             YU, ZA, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                            AU 2001-32036
                                20010820
     AU 2001032036
                          Α5
                                                                    20010208
     EP 1254119
                                            EP 2001-904117
                          A1
                                20021106
                                                                    20010208
     EP 1254119
                          В1
                                20060412
             AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
                                            JP 2001-558432
     JP 2003522761
                          T2
                                20030729
                                                                    20010208
                                            AT 2001-904117
     AT 323072
                          E
                                20060415
                                                                    20010208
     TW 230705
                          B1
                                20050411
                                            TW 2001-90104533
                                                                    20010227
     US 2003109538
                          A1
                                20030612
                                            US 2002-182788
                                                                    20020731
     US 6780870
                          B2
                                20040824
PRAI GB 2000-3224
                          Α
                                20000211
     WO 2001-GB511
                                20010208
     MARPAT 135:180777
OS
AB
     The title compds. [I; R1, R2 = H, alkyl; R3 = alkyl, NH2; R4 = H, alkyl; A
     = 5-6 membered aryl, 5-6 membered aryl substituted by one or more R5; R5 =
     halo, alkyl, alkoxy, etc.; n = 1-4] which are potent and selective
     inhibitors of COX-2 and are of use in the treatment of the pain, fever,
     inflammation of a variety of conditions and diseases, were prepared and
     formulated. E.g., a multi-step synthesis of the pyrimidinamine I [R1, R2
     = H; R3 = Me; R4 = H; A = 4-pyridyl; n = 1] which showed IC50 of 1.3 nM
     against COX-2, was given.
IT
     354806-68-1P 354806-72-7P 354806-73-8P
     354806-74-9P 354806-75-0P 354806-76-1P
     354806-77-2P 354806-78-3P 354806-79-4P
     354806-80-7P 354806-81-8P 354806-82-9P
     354806-83-0P 354806-84-1P 354806-85-2P
     354806-86-3P 354806-89-6P 354806-90-9P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of 2-pyrimidinamines as selective inhibitors of COX-2)
RN
     354806-68-1 CAPLUS
CN
     2-Pyrimidinamine, 4-[4-(methylsulfonyl)phenyl]-N-(phenylmethyl)-6-
     (trifluoromethyl) - (9CI) (CA INDEX NAME)
```

RN 354806-72-7 CAPLUS

CN 2-Pyrimidinamine, N-[(4-methoxyphenyl)methyl]-4-[4-(methylsulfonyl)phenyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 354806-73-8 CAPLUS

CN 2-Pyrimidinamine, 4-[4-(methylsulfonyl)phenyl]-N-[[4-(trifluoromethoxy)phenyl]methyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & CF_3 \\ \hline \\ O & NH-CH_2 \end{array}$$

RN 354806-74-9 CAPLUS

CN 2-Pyrimidinamine, N-[(3,4-difluorophenyl)methyl]-4-[4-(methylsulfonyl)phenyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$Me^{-\frac{O}{S}}$$

$$O$$

$$NH-CH_2$$

RN 354806-75-0 CAPLUS

CN 2-Pyrimidinamine, 4-[4-(methylsulfonyl)phenyl]-6-(trifluoromethyl)-N-[[4-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 354806-76-1 CAPLUS

CN 2-Pyrimidinamine, N-[(4-methylphenyl)methyl]-4-[4-(methylsulfonyl)phenyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 354806-77-2 CAPLUS

CN 2-Pyrimidinamine, N-[(3-fluorophenyl)methyl]-4-[4-(methylsulfonyl)phenyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$Me^{-S}$$

$$0$$

$$NH-CH_2$$

RN 354806-78-3 CAPLUS

CN 2-Pyrimidinamine, N-[(4-fluorophenyl)methyl]-4-[4-(methylsulfonyl)phenyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 354806-79-4 CAPLUS

CN 2-Pyrimidinamine, N-[(3,5-difluorophenyl)methyl]-4-[4- (methylsulfonyl)phenyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 354806-80-7 CAPLUS

CN 2-Pyrimidinamine, N-[(2,5-difluorophenyl)methyl]-4-[4-(methylsulfonyl)phenyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$Me - S \qquad CF3 \qquad F \qquad NH - CH2 \qquad F$$

RN 354806-81-8 CAPLUS

CN 2-Pyrimidinamine, N-[(2,6-difluorophenyl)methyl]-4-[4-(methylsulfonyl)phenyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$Me - S \qquad CF3 \qquad F \qquad NH - CH2 \qquad F$$

RN 354806-82-9 CAPLUS

CN 2-Pyrimidinamine, N-[(2,4-difluorophenyl)methyl]-4-[4-(methylsulfonyl)phenyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$Me - S \longrightarrow N \longrightarrow NH - CH_2 \longrightarrow F$$

RN 354806-83-0 CAPLUS

CN 2-Pyrimidinamine, N-[[4-(difluoromethoxy)phenyl]methyl]-4-[4-(methylsulfonyl)phenyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

$$Me - S = O - CHF_2$$

$$O = N$$

$$NH - CH_2$$

RN 354806-84-1 CAPLUS

CN 2-Pyrimidinamine, N-[(3-methylphenyl)methyl]-4-[4-(methylsulfonyl)phenyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 354806-85-2 CAPLUS

CN 2-Pyrimidinamine, N-[(2-fluorophenyl)methyl]-4-[4-(methylsulfonyl)phenyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 354806-86-3 CAPLUS

CN 2-Pyrimidinamine, N-[(3-chlorophenyl)methyl]-4-[4-(methylsulfonyl)phenyl]-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 354806-89-6 CAPLUS

CN 2-Pyrimidinamine, N-methyl-4-[4-(methylsulfonyl)phenyl]-N-(phenylmethyl)-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 354806-90-9 CAPLUS

CN 2-Pyrimidinamine, 4-[4-(methylsulfonyl)phenyl]-N-(3-phenylpropyl)-6-(trifluoromethyl)-(9CI) (CA INDEX NAME)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/671,070

ANSWER 75 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN L10

AN 2001:235559 CAPLUS

DN 134:266319

ΤI CD40 function inhibitors containing (hetero)aryl compounds and their preparation

Saito, Shoichi; Akane, Katsura; Fujimoto, Katsumi; Shiraishi, Akio; TN Kurakata, Shinichi; Maeda, Hiroaki; Tatsuta, Toru

Sankyo Co., Ltd., Japan PΑ

Jpn. Kokai Tokkyo Koho, 139 pp. SO

CODEN: JKXXAF

DΤ Patent

Japanese LA

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 2001089452 PRAI JP 1999-267909	A2	20010403 19990922	JP 1999-267909	19990922

MARPAT 134:266319 OS

AR Title inhibitors, useful for prevention and treatment of allergy, rheumatoid, autoimmune disease, and arteriosclerosis, contain aromatic compds. I [R1, R3, R4 = H, OH, halo, C1-15 alkyl(oxy), C1-15 alkylthio, (un) substituted (hetero) aryl, etc.; R2 = NO2, nitrile, CO2H, C2-6 alkoxycarbonyl; R1CCR2 may form (un)substituted (hetero)aryl; X, Y = N, CH] or their salts as active ingredients. Thus, MeOCPh:C(CO2Et)2 was refluxed with benzamidine HCl salt and NaH in EtOH for 5 h, evaporated, neutralized, extracted with AcOEt, the organic phase concentrated, and treated

with

POC13 and morpholine to give 52% I (R1 = R4 = Ph, R2 = CO2Et, R3 = 4-morpholino, X = Y = N), which at 25 μ M inhibited 88% formation of IL-12.

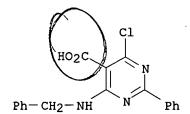
IT 332071-66-6P

> RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of (hetero) aryl compds. as CD40 function inhibitors)

RN 332071-66-6 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-chloro-2-phenyl-6-[(phenylmethyl)amino]-, monosodium salt (9CI) (CA INDEX NAME)



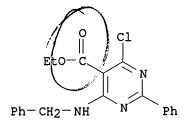
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IT 332072-06-7

> RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of (hetero)aryl compds. as CD40 function inhibitors)

RN 332072-06-7 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-chloro-2-phenyl-6-[(phenylmethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)



```
ANSWER 76 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
L10
AN
     2000:861658 CAPLUS
DN
     134:29425
ΤI
     Novel 4-phenyl-pyrimidine derivatives as NK-1 receptor antagonists
     Boes, Michael; Galley, Guido; Godel, Thierry; Hoffmann, Torsten; Hunkeler,
     Walter; Schnider, Patrick; Stadler, Heinz
PA
     F. Hoffmann-La Roche A.-G., Switz.
     PCT Int. Appl., 64 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     English
LА
FAN.CNT 1
     PATENT NO.
                          KIND
                                 DATE
                                              APPLICATION NO.
                                                                      DATE
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PI
     WO 2000073279
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                                                                      20000524
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             JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG,
             MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL,
             TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
             DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ,
             CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     US 6274588
                                              US 2000-575382
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                                 20060208
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     TR 200103457
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                                              TR 2001-3457
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     JP 2003500478
                           T2
                                 20030107
                                              JP 2000-621345
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     JP 3590592
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                                 20041117
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                                 20040304
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     NZ 515407
                           Α
                                 20040326
                                              NZ 2000-515407
                                                                      20000524
     RU 2243221
                           C2
                                 20041227
                                              RU 2001-133458
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                                 20060215
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     ZA 2001009163
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                                 20030206
                                              ZA 2001-9163
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     NO 2001005700
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                                 20011122
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                                                                      20011122
     NO 321354
                           В1
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     HR 2001000871
                           A1
                                 20030430
                                              HR 2001-871
                                                                      20011122
     HK 1046528
                           A1
                                 20050225
                                              HK 2002-107643
                                                                      20021022
PRAI EP 1999-110483
                                 19990531
                           Α
     WO 2000-EP4701
                           W
                                 20000524
os
     MARPAT 134:29425
AΒ
     The invention discloses pyrimidine derivs. I [R1 = H or halo; R2 = H,
     halo, lower alkyl or lower alkoxy; R1 and R2 may be together with the two
     carbon atoms -CH=CH-CH=CH-; R3 = halo, CF3, lower alkyl or lower alkoxy;
     R4, R6 = (independently) H or lower alkyl; R5 = lower alkyl, lower alkoxy,
     amino, Ph, hydroxy-lower alkyl, cyano-lower alkyl, carbamoyl-lower alkyl,
     pyridyl, pyrimidyl, (un) substituted - (CH2) n-piperazinyl, which is
     optionally substituted by one or two lower alkyl groups or by
     hydroxy-lower alkyl, -(CH2)n-morpholinyl, -(CH2)n-piperidinyl, -(CH2)n+1-imidazolyl, lower alkyl-sulfanyl, lower alkyl-sulfonyl,
     benzylamino, -NH-(CH2)n+1N(R7)2, -(CH2)n+1N(R7)2, -O-(CH2)n+1-morpholinyl,
     -O-(CH2)n+1-piperidinyl or -O-(CH2)n+1N(R7)2, wherein R7 = H or lower
     alkyl; n = 0-2; X = -C(0)N(R7) - or -N(R7)C(0) and their pharmaceutically
```

acceptable acid addition salts as NK-1 receptor antagonists. The preferred compds. exhibited pKi values for NK-1 receptor affinity in the range of 8.00-9.20, e.g., the pKi of II was 8.45. With demonstrated affinity to the NK-1 receptor, these compds. may prove useful for the treatment of medical conditions related to this receptor, e.g., inflammatory conditions such as arthritis, migraine, asthma, etc., and in particular CNS disorders such as depression or emesis.

IT 311339-73-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn and biol. activity of phenylpyrimidine derivs. as NK-1 antagonists)

RN 311339-73-8 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[[3,5-bis(trifluoromethyl)phenyl]methyl]-N-methyl-4-phenyl-2-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L10 ANSWER 77 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 2000:217698 CAPLUS
- DN 133:2300
- TI Identification of Cryptosporidium parvum dihydrofolate reductase inhibitors by complementation in Saccharomyces cerevisiae
- AU Brophy, Victoria Hertle; Vasouez, John; Nelson, Richard G.; Forney, John R.; Rosowsky, Andre; Sibley, Carol Hopkins
- CS Department of Genetics, University of Washington, Seattle, WA, 98195-7360, USA
- SO Antimicrobial Agents and Chemotherapy (2000), 44(4), 1019-1028 CODEN: AMACCO; ISSN: 0066-4804
- PB American Society for Microbiology
- DT Journal
- LA English
- AB There is a pressing need for drugs effective against the opportunistic protozoan pathogen Cryptosporidium parvum. Folate metabolic enzymes and enzymes of the thymidylate cycle, particularly dihydrofolate reductase (DHFR), have been widely exploited as chemotherapeutic targets. Although many DHFR inhibitors have been synthesized, only a few have been tested against C. parvum. To expedite and facilitate the discovery of effective anti-Cryptosporidium antifolates, the authors have developed a rapid and facile method to screen potential inhibitors of C. parvum DHFR using the model eukaryote, Saccharomyces cerevisiae. They expressed the DHFR genes of C. parvum, Plasmodium falciparum, Toxoplasma gondii, Pneumocystis carinii, and humans in the same DHFR-deficient yeast strain and observed that each heterologous enzyme complemented the yeast DHFR deficiency. In this work, the authors describe their use of the complementation system to screen known DHFR inhibitors and their discovery of several compds. that inhibited the growth of yeast reliant on the C. parvum enzyme. These same compds. were also potent or selective inhibitors of the purified recombinant C. parvum DHFR enzyme. Six novel lipophilic DHFR inhibitors potently inhibited the growth of yeast expressing C. parvum DHFR. However, the inhibition was nonselective, as these compds. also strongly inhibited the growth of yeast dependent on the human enzyme. Conversely, the antibacterial DHFR inhibitor trimethoprim and two close structural analogs were highly selective, but weak, inhibitors of yeast complemented by the C. parvum enzyme. Future chemical refinement of the potent and selective lead compds. identified in this study may allow the design of an efficacious antifolate drug for the treatment of cryptosporidiosis.
- IT 35960-68-0
 - RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
 - (identification of Cryptosporidium parvum dihydrofolate reductase inhibitors by complementation in Saccharomyces cerevisiae)
- RN 35960-68-0 CAPLUS
- CN L-Glutamic acid, N-[4-[[3-(2-amino-1,4-dihydro-4-oxo-6-phenyl-5-pyrimidinyl)propyl]amino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 66 THERE ARE 66 CITED REFERENCES—AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 78 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
ΑN
     2000:115763 CAPLUS
DN
     132:151833
ΤI
     Preparation of 4-amino-2-arylpyrimidines as modulators of cyclic quanosine
     monophosphate production.
IN
     Schindler, Ursula; Schoenafinger, Karl; Strobel, Hartmut
PA
     Hoechst Marion Roussel Deutschland G.m.b.H., Germany
so
     Ger. Offen., 22 pp.
     CODEN: GWXXBX
DT
     Patent
LΑ
     German
FAN.CNT 1
     PATENT NO.
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                                             APPLICATION NO.
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PΙ
     DE 19836697
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             IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG,
             MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL,
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     AU 9957307
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                          A1
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     JP 2002522536
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                                 20031216
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PRAI DE 1998-19836697
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     WO 1999-EP5636
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                                19990804
os
     MARPAT 132:151833
AB
     Title compds. [I; R1 = (substituted) alkyl, cycloalkyl, 5-7 membered
     heterocyclyl; R2 = H, (substituted) alkyl, cycloalkyl, 5-7 membered
     heterocyclyl; R1R2N = (substituted) 5-7 membered heterocyclyl; R3 = aryl;
     R4 = alkyl, CF3, aryl], were prepared Thus, 4-chloro-2(4-chlorophenyl)-6-
     isopropylpyrimidine (preparation given) and 4-amino-2,2,6,6,-
     tetramethylpiperidine were stirred at 150° for 2 h to give
     2-(4-chlorophenyl)-6-isopropyl-4-[(2,2,6,6-tetramethylpiperidin-4-
     yl)amino]pyrimidine dihydrochloride. Tested I at 50 µM stimulated
     guanylate cyclase by >4 to 28-fold.
     257948-67-7P 257948-73-5P 257948-92-8P
ΙT
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of 4-amino-2-arylpyrimidines as modulators of cyclic guanosine
       monophosphate production)
RN
     257948-67-7 CAPLUS
     4-Pyrimidinamine, 2-(4-chlorophenyl)-N-[2-(3-methoxyphenyl)ethyl]-6-(1-
CN
```

methylethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 257948-73-5 CAPLUS

CN 4-Pyrimidinamine, 2-(4-chlorophenyl)-6-(1-methylethyl)-N-(phenylmethyl)-(9CI) (CA INDEX NAME)

RN 257948-92-8 CAPLUS

CN 4-Pyrimidinamine, 2-(4-chlorophenyl)-N-[2-(3-methoxyphenyl)ethyl]-6-phenyl, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

IT 257949-74-9

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

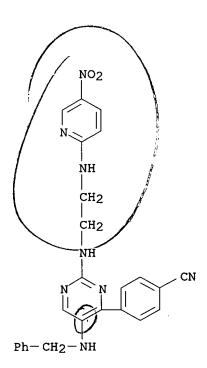
(preparation of 4-amino-2-arylpyrimidines as modulators of cyclic quanosine

monophosphate production)

RN 257949-74-9 CAPLUS

CN 4-Pyrimidinamine, 2-(4-chlorophenyl)-N-ethyl-6-(1-methylethyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

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ANSWER 79 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
L10
     1999:811233 CAPLUS
AN
DN
     132:64265
     Preparation of aminopyrimidines and -pyridines as glycogen synthase kinase
TI
     3 inhibitors
    Nuss, John M.; Harrison, Stephen D.; Ring, David B.; Boyce, Rustum S.;
IN
     Brown, Sean P.; Goff, Dane; Johnson, Kirk; Pfister, Keith B.; Ramurthy,
     Savithry; Renhowe, Paul A.; Seely, Lynn; Subramanian, Sharadha; Wagman,
     Allan S.; Zhou, Xiaohui A.
     Chiron Corporation, USA
PA
SO
     PCT Int. Appl., 262 pp.
     CODEN: PIXXD2
DT
     Patent
     English
LA
FAN.CNT 3
                                                                    DATE
     PATENT NO.
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                                DATE
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                                                                    19990618
     JP 2003527303
                          T2
                                20030916
                                            JP 2000-554722
     AT 274510
                                20040915
                                            AT 1999-933522
                                                                    19990618
                                20030710
                                            US 2002-309535
                                                                    20021203
     US 2003130289
                          A1
     US 7037918
                          В2
                                20060502
PRAI US 1998-89978P
                          Ρ
                                19980619
     US 1999-336098
                          Α3
                                19990618
     WO 1999-US13809
                                19990618
                          W
     MARPAT 132:64265
os
     RZCR2R12CR3R13Z1R5 [I; R = (un)substituted (hetero)aryl; Z = O, NR1,
AB
     CR1R11; Z1 = O, NR4, CR4R14; R1-R4 = H, OH, NH2, alkyl, alkoxy, etc.; R5 =
     (un) substituted 2-pyridyl or -pyrimidyl; R11-R14 = H or alkyl] were prepared
     Thus, 2-chloro-5-nitropyridine was aminated by H2N(CH2)3NH2 and the
     product N-acylated by benzotriazolecarboxamidinium tosylate to give the
     alkylguanidine which was cyclocondensed with resin-bound
     4-(MeCO)C6H4CONHCH2C6H4Br-3 and Cs2CO3 to give, after resin cleavage,
     title compound II. Data for biol. activity of I were given.
IT
     252904-40-8P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of aminopyrimidines and -pyridines as glycogen synthase kinase
        3 inhibitors)
RN
     252904-40-8 CAPLUS
     Benzonitrile, 4-[2-[[2-[(5-nitro-2-pyridinyl)amino]ethyl]amino]-5-
CN
     [(phenylmethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)
```



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

10/671,070

L10 ANSWER 80 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1999:729784 CAPLUS

DN 132:308303

TI Synthesis and preliminary study of anticonvulsive activity of 4-substituted amino-6-phenylpyrimidines

AU Zhang, Xiaohui; Wang, Donghui; Chen, Naiyong; Tao, Cheng

CS Institute of Applied Pharmacy Science, Beijing Medical Univ., Beijing, 100083, Peop. Rep. China

SO Zhongguo Yaowu Huaxue Zazhi (1999), 9(3), 192-195 CODEN: ZYHZEF; ISSN: 1005-0108

PB Zhongguo Yaowu Huaxue Zazhi Bianjibu

DT Journal

LA Chinese

AB Seven 4-substituted amino-6-phenylpyrimidines were designed and synthesized, and their anticonvulsive activities were studied. All the synthetic compds. showed some anticonvulsive activity, 4-benzylamino-6-phenylpyrimidine showed strong effects, even stronger than dilantin sodium. Structure-activity relationship was discussed.

IT 266303-86-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and anticonvulsant activity of 4-substituted amino-6-phenylpyrimidines)

RN 266303-86-0 CAPLUS

CN 4-Pyrimidinamine, 6-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 81 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1999:583185 CAPLUS

DN 131:199710

TI Preparation of nitrogen containing aromatic compounds as herbicides

IN Kuboyama, Nobuhiro; Koizumi, Kazuya; Yamashita, Osamu; Wakabayashi, Osamu; Tomono, Kotaro; Hattori, Takashi

PA Tomono Agrica K. K., Japan

SO Jpn. Kokai Tokkyo Koho, 42 pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

PATENT NO.		KIND DATE		APPLICATION NO.	DATE	
PI JP	11246528	A2	19990914	JP 1998-345843	19981204	
PRAI JP	1997-335223	Α	19971205			

OS MARPAT 131:199710

Title compds. [I; X, Y, Z are independently N, CH; R = CF3; R1 = CH3, H, CH2CH3, (CH3)2CH, C6H5; A = NH, NCHO, NCOCH3, NCOCH2CH3, NCOCH2CH2CH3, NCOCH(CH3)2, NCOC(CH3)3, O, NCH2CCH, S; B = CH2, (S)-CH3CH, (R)-CH3CH, CH3CH, CH3CHCH2CH2, (CH3)2CCH2, (CH2)4, (CH2)2, (CH2)3; R2 = 4-ClC6H4, 2-ClC6H4, 3-ClC6H4, 4-BrC6H4, 3-F3CC6H4, 4-F3CC6H4, 2-BrC6H4, 3-BrC6H4, 3-Br-4-FC6H3, 2-CH3C6H4, 3-O2NC6H4, 2-HOC6H4, C6H5, 2-pyridyl, 3-pyridyl, cyclohexyl; BR2 = (CH2)7CH3, (CH2)2CH(C6H5)2; etc.], and salts are prepared as herbicides and tested on rice paddies. Thus, the title compound I (R = CF3; R1 = CH3; A = NH; B = CH2; R2 = 4-ClC6H4; X = N; Y = N; Z = CH) was prepared

IT 241162-08-3P 241163-03-1P 241163-09-7P 241163-10-0P 241163-11-1P 241163-12-2P 241163-13-3P 241163-68-8P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of nitrogen containing aromatic compds. as herbicides)

RN 241162-08-3 CAPLUS

CN 4-Pyrimidinamine, N-[(4-chlorophenyl)methyl]-2-phenyl-6-(trifluoromethyl)(9CI) (CA INDEX NAME)

RN 241163-03-1 CAPLUS

CN Formamide, N-[(4-chlorophenyl)methyl]-N-[2-phenyl-6-(trifluoromethyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 241163-09-7 CAPLUS

CN Formamide, N-[(2-chlorophenyl)methyl]-N-[2-phenyl-6-(trifluoromethyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 241163-10-0 CAPLUS

CN Formamide, N-[(3-chlorophenyl)methyl]-N-[2-phenyl-6-(trifluoromethyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 241163-11-1 CAPLUS

CN Formamide, N-[(2-methylphenyl)methyl]-N-[2-phenyl-6-(trifluoromethyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 241163-12-2 CAPLUS

CN Formamide, N-[(3-methylphenyl)methyl]-N-[2-phenyl-6-(trifluoromethyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 241163-13-3 CAPLUS

CN Formamide, N-[(4-methylphenyl)methyl]-N-[2-phenyl-6-(trifluoromethyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 241163-68-8 CAPLUS

CN 4-Pyrimidinamine, 2-phenyl-N-(4-phenylbutyl)-6-(trifluoromethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 82 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

1999:387716 CAPLUS AN

DN 131:78466

Adenosine A3 antagonists ΤI

Sugiura, Yoshihiro; Miwatari, Seiji; Kimura, Hiroyuki; Knzaki, Naoyuki

Takeda Chemical Industries, Ltd., Japan PA

Jpn. Kokai Tokkyo Koho, 30 pp. SO

CODEN: JKXXAF

DTPatent

LΑ Japanese

FAN. CNT 1

	PATENT NO.		DATE	APPLICATION NO.	DATE	
PI	JP 11158073	A2	19990615	JP 1998-270755	19980925	
PRAI	JP 1997-262525	Α	19970926			

PRAI JP 1997-262525

MARPAT 131:78466

AΒ Adenosine A3 receptor antagonists contain (un) substituted amino-substituted N2-3-containing heterocyclic [5-8 ring-containing] compds.

such

as 2-chloro-4-ethylamino-6-phenylamino-1,3,5-triazine and 2,4-bis[phenylamino]-6-cyclohexylamino-1,3,5-triazine. Of 6 compds. tested, the IC50 values of adenosine A3 receptor antagonist activities ranged from 0.7 to 285.9 nM as determined in human adenosine A3 receptor-expressing plasmid-transformed CHO (dhfr-) cell cultures. Tablets were formulated containing 2,4-bis[phenylamino]-6-cyclohexylamino-1,3,5-triazine 50, lactose 34, corn starch 10.6, corn starch paste 5, magnesium stearate 0.4 and calcium CM-cellulose 20 mg. The drugs are useful for treating e.g. brain ischemic disease.

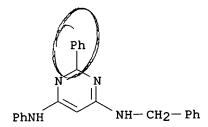
IT 228575-16-4

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES

(adenosine A3 receptor antagonists and pharmaceutical compns.)

RN 228575-16-4 CAPLUS

4,6-Pyrimidinediamine, N,2-diphenyl-N'-(phenylmethyl)- (9CI) (CA INDEX CN NAME)



```
ANSWER 83 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
     1998:788746 CAPLUS
AN
DN
     130:52406
ΤI
     Substituted biphenyl isoxazole sulfonamides useful as endothelin
     antagonists
     Murugesan, Natesan; Barrish, Joel C.; Spergel, Steven H.
IN
PA
     Bristol-Myers Squibb Co., USA
SO
     U.S., 107 pp., Cont.-in-part of U.S. Ser. No. 754,715, abandoned.
     CODEN: USXXAM
DT
     Patent
LΑ
     English
FAN.CNT 2
     PATENT NO.
                           KIND
                                   DATE
                                                 APPLICATION NO.
                                                                           DATE
                                                 _____
ΡI
     US 5846990
                            Α
                                   19981208
                                                 US 1997-799616
                                                                           19970213
     TW 517057
                            В
                                                 TW 1997-86101898
                                   20030111
                                                                           19970218
     ZA 9701423
                                                 ZA 1997-1423
                            Α
                                    19980819
                                                                           19970219
     CA 2240043
                                    19970821
                                                 CA 1997-2240043
                            AΑ
                                                                           19970220
     WO 9729748
                            A1
                                                 WO 1997-US3956
                                    19970821
                                                                           19970220
         W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE,
              ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, AM, AZ, BY, KG,
              KZ, MD, RU, TJ, TM
         RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML,
              MR, NE, SN, TD, TG
     AU 9722098
                             A1
                                    19970902
                                                 AU 1997-22098
                                                                           19970220
     AU 720458
                             B2
                                    20000601
     EP 921800
                             A1
                                    19990616
                                                 EP 1997-915055
                                                                           19970220
     EP 921800
                             В1
                                    20040414
              AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
              IE, FI
     JP 2002500619
                            T2
                                   20020108
                                                 JP 1997-529620
                                                                           19970220
     AT 264324
                            E
                                   20040415
                                                 AT 1997-915055
                                                                           19970220
     ES 2219762
                            Т3
                                   20041201
                                                 ES 1997-915055
                                                                           19970220
PRAI US 1995-493331
                            B2
                                   19950724
     US 1996-603975
                            В1
                                   19960220
     US 1996-754715
                            B2
                                   19961121
     US 1997-799616
                            Α
                                   19970213
     WO 1997-US3956
                            W
                                   19970220
OS
     MARPAT 130:52406
AB
     Title compds. I inhibit the activity of endothelin (no data), and are
     useful as antihypertensives, etc. The symbols in I are defined as follows
     [one of X and Y = N, other = O; J = O, S, N, (un)substituted NH; K, L = N
     or C, provided that at least one is C; p = 0-2; R1-R4 (bound to ring C
     atoms) = H, (un)substituted alkyl, alkenyl, alkynyl, alkoxy, cycloalkyl,
     cycloalkylalkyl, cycloalkenyl, cycloalkenylalkyl, aryl, aryloxy, aralkyl,
     aralkoxy, halo, OH, cyano, NO2, CHO, etc.; or R3R4 = (un)substituted
     alkylene or alkenylene; R5-R8 = groups similar to R1-R4, plus
     heterocyclyl, heterocyclyloxy, and others]. Over 280 synthetic examples are given. For instance, the MEM-protected, isoxazole-containing bromide II
     [R = Br] was lithiated, treated with B(OPr-iso)3, and hydrolyzed to give
     82% II [R = B(OH)2]. The latter was coupled with 2-(4-bromophenyl)oxazole
     using Pd(PPh3)4 catalyst (70%), followed by acidic deprotection of the MEM
```

IT 195446-58-3P

group (52%), to give title compound III.

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of substituted biphenyl isoxazole sulfonamides as endothelin antagonists)

RN 195446-58-3 CAPLUS

CN [1,1'-Biphenyl]-2-sulfonamide, 2'-[[[4-(4-chlorophenyl)-6-ethoxy-2-pyrimidinyl]amino]methyl]-N-(3,4-dimethyl-5-isoxazolyl)-4'-(2-oxazolyl)-(9CI) (CA INDEX NAME)

PAGE 1-A

Me NH-S

Me NH-S

NH-S

NH-S

NH-S

NH-S

NH-S

NH-S

RE.CNT 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 84 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
L10
AN
     1998:197493 CAPLUS
DN
     128:217383
ΤI
     Preparation of pyrimidine compounds as pesticides
     Hamamoto, Isami; Ishimitsu, Keiichi; Ihori, Yoichi; Takahashi, Hidemitsu;
IN
     Nakamura, Takehiko; Iwasa, Takao
PA
     Nippon Soda Co., Ltd., Japan
     PCT Int. Appl., 55 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     Japanese
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                    DATE
                         ____
PΙ
                                19980326
                                            WO 1997-JP3292
                                                                    19970918
     WO 9812184
                          A1
         W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,
             DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KR, KZ, LC, LK,
             LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO,
             RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM,
             AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR,
             GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA,
             GN, ML, MR, NE, SN, TD, TG
                                            AU 1997-42217
                                                                    19970918
     AU 9742217
                          A1
                                19980414
PRAI JP 1996-269309
                                19960919
                          Α
     JP 1996-356867
                                19961226
                          Α
     WO 1997-JP3292
                                19970918
                          W
     MARPAT 128:217383
os
     The title compds. (I; R1-R5, R8-R12 = H, halo, C1-6 alkyl, haloalkyl,
AΒ
     alkoxy, alkylthio, or haloalkoxy, etc.; R6, R7 = H, halo, C1-6 alkyl or
     haloalkyl; R13 = H, optionally substituted C1-6 alkyl, C2-6 alkenyl, or
     alkynyl, optionally substituted carbamoyl, etc.) are prepared I are useful
     as pesticides. Thus, 4-chloro-6-(4-fluoro-3-trifluoromethylphenoxy)pyrimi
     dine (preparation given) was reacted with 4-fluoro-3-trifluoromethylaniline in
     the presence of Et3N to give 67% the title compound (II). II at 125 ppm
     showed 100% insecticidal effect for Pseudaletia separata after 6 days.
IT
     204121-40-4P
     RL: AGR (Agricultural use); BAC (Biological activity or effector, except
     adverse); BSU (Biological study, unclassified); SPN (Synthetic
     preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of pyrimidine compds. as pesticides)
RN
     204121-40-4 CAPLUS
     4-Pyrimidinamine, N-[(4-chlorophenyl)methyl]-N,6-bis(4-fluoro-3-
CN
     (trifluoromethyl)phenyl] - (9CI) (CA INDEX NAME)
   F<sub>3</sub>C
                         CF3
```

Page 595

10/671,070

L10 ANSWER 85 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1998:136037 CAPLUS

DN 128:244022

TI Synthesis and transformations of methyl (E)-2-(acetylamino)-3-cyanoprop-2-enoate and methyl (E)-2-(benzoylamino)-3-cyanoprop-2-enoate, versatile reagents for the preparation of polyfunctional heterocyclic systems

AU Pizzioli, Lucija; Ornik, Brina; Svete, Jurij; Stanovnik, Branko

CS Fac. Chem. Chem. Technol., Univ. Ljubljana, Ljubljana, 1000, Slovenia

SO Helvetica Chimica Acta (1998), 81(2), 231-235 CODEN: HCACAV; ISSN: 0018-019X

PB Verlag Helvetica Chimica Acta AG

DT Journal

LA English

OS CASREACT 128:244022

AB The title compds. were prepared from the corresponding (Z)-2-(acylamino)-3-(dimethylamino)propenoates. The compds. proved to be versatile synthons for the synthesis of polysubstituted heterocyclic systems such as pyrroles, pyrimidines, pyridazines, pyrazoles, and isoxazoles.

IT 204767-43-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of polyfunctional heterocyclic compds. from
 (acylamino)cyanopropenoates)

RN 204767-43-1 CAPLUS

CN 4-Pyrimidinecarboxamide, 2-phenyl-N-(phenylmethyl)-6-[(phenylmethyl)amino]-(9CI) (CA INDEX NAME)

```
ANSWER 86 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     1997:557640 CAPLUS
DN
     127:248103
ΤI
     Substituted biphenyl isoxazole sulfonamides useful as endothelin
     antagonists
ΙN
     Murugesan, Natesan; Barrish, Joel C.; Spergel, Steven H.
PΑ
     Bristol-Myers Squibb Company, USA
SO
     PCT Int. Appl., 325 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 2
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                    DATE
                         ----
                                _____
                                            ______
PΙ
     WO 9729748
                          A1
                                19970821
                                            WO 1997-US3956
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        W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE,
             ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR,
             LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD,
             SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN, AM, AZ, BY, KG,
             KZ, MD, RU, TJ, TM
         RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR,
             IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML,
             MR, NE, SN, TD, TG
     US 5846990
                          Α
                                19981208
                                            US 1997-799616
                                                                    19970213
     TW 517057
                          В
                                20030111
                                            TW 1997-86101898
                                                                    19970218
                                            ZA 1997-1423
     ZA 9701423
                          Α
                                19980819
                                                                    19970219
     AU 9722098
                                19970902
                                            AU 1997-22098
                          A1
                                                                    19970220
     AU 720458
                          B2
                                20000601
     EP 921800
                                19990616
                          A1
                                            EP 1997-915055
                                                                    19970220
     EP 921800
                          В1
                                20040414
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, FI
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                                20020108
                                            JP 1997-529620
                                                                    19970220
     AT 264324
                          E
                                20040415
                                            AT 1997-915055
                                                                    19970220
PRAI US 1996-603975
                          Α
                                19960220
     US 1996-754715
                          Α
                                19961121
     US 1997-799616
                         A.
                                19970213
     US 1995-493331
                          B2
                                19950724
     WO 1997-US3956
                          W
                                19970220
OS
     MARPAT 127:248103
AB
     Title compds. I inhibit the activity of endothelin (no data), and are
     useful as antihypertensives, etc. The symbols in I are defined as follows
     [one of X and Y = N, other = O; J = O, S, N, (un)substituted NH; K, L = N
     or C, provided that at least one is C; p = 0-2; R1-R4 (bound to ring C
     atoms) = H, (un)substituted alkyl, alkenyl, alkynyl, alkoxy, cycloalkyl,
     cycloalkylalkyl, cycloalkenyl, cycloalkenylalkyl, aryl, aryloxy, aralkyl,
     aralkoxy, halo, OH, cyano, NO2, CHO, etc.; or R3R4 = (un)substituted
     alkylene or alkenylene; R5-R8 = groups similar to R1-R4, plus
     heterocyclyl, heterocyclyloxy, and others]. Over 280 synthetic examples
     are given. For instance, the MEM-protected, isoxazole-containing bromide II
     [R = Br] was lithiated, treated with B(OPr-iso)3, and hydrolyzed to give
     82% II [R = B(OH)2]. The latter was coupled with 2-(4-bromophenyl)oxazole
     using Pd(PPh3)4 catalyst (70%), followed by acidic deprotection of the MEM
     group (52%), to give title compound III.
IT
     195446-58-3P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
```

BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of substituted biphenyl isoxazole sulfonamides as endothelin antagonists)

RN 195446-58-3 CAPLUS

CN [1,1'-Biphenyl]-2-sulfonamide, 2'-[[[4-(4-chlorophenyl)-6-ethoxy-2-pyrimidinyl]amino]methyl]-N-(3,4-dimethyl-5-isoxazolyl)-4'-(2-oxazolyl)-(9CI) (CA INDEX NAME)

OET

NH

CH2

R

PAGE 1-A

L10 ANSWER 87 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

1997:407610 CAPLUS AN

DN 127:121691

Synthesis of 4,6-disubstituted and 4,5,6-trisubstituted TI 2-phenylpyrimidines and their affinity towards Al adenosine receptors

Biagi, Giuliana; Giorgi, Irene; Livi, Oreste; Scartoni, Valerio; ΑU Lucacchini, Antonio

Dip. Scienze Farmaceutiche, Univ. Pisa, Pisa, 56126, Italy CS

SO Farmaco (1997), 52(1), 61-65 CODEN: FRMCE8; ISSN: 0014-827X

Societa Chimica Italiana PB

DTJournal

LA English

The preparation and assay of the title compds., e.g., I (R = cyclohexyl, AΒ pentyl), are reported. The results support our hypothesis about the possibility that mols. characterized by great flexibility, such as 2-phenyl-4,5,6-triaminopyrimidines, can better interact with the receptor sites than rigid mols. such as 2,6,9-trisubstituted 8-azaadenines. The relatively low activity shown by pyrimidine derivs. demonstrated the importance of the bicyclic aromatic system in 8-azaadenines and adenines for a favorable interaction with the Al adenosine receptors.

192631-72-4P 192631-73-5P 192631-74-6P IT

192631-75-7P 192631-86-0P 192631-87-1P

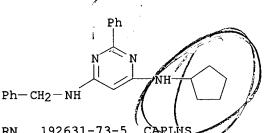
192631-88-2P 192631-89-3P 192631-94-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of 4,6-disubstituted and 4,5,6-trisubstituted 2-phenylpyrimidines and their Al adenosine receptor affinity)

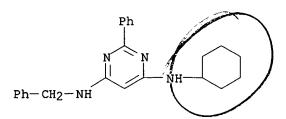
RN 192631-72-4 CAPLUS

4,6-Pyrimidinediamine, N-cyclopentyl-2-phenyl-N'-(phenylmethyl)- (9CI) CN (CA INDEX NAME)



192631-73-5 RN

4,6-Pyrimidinediamine, N-cyclohexyl-2-phenyl-N'-(phenylmethyl)- (9CI) (CA CN INDEX NAME)



RN 192631-74-6 CAPLUS

4,6-Pyrimidinediamine, N-butyl-2-phenyl-N'-(phenylmethyl)- (9CI) (CA CN INDEX NAME)

RN 192631-75-7 CAPLUS

CN 4,6-Pyrimidinediamine, N-pentyl-2-phenyl-N'-(phenylmethyl)- (9CI) (CA INDEX NAME)

Me- (CH₂)
$$_4$$
-NH NH-CH₂-Ph

RN 192631-86-0 CAPLUS

CN 4,5,6-Pyrimidinetriamine, N4-cyclopentyl-2-phenyl-N6-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 192631-87-1 CAPLUS

CN 4,5,6-Pyrimidinetriamine, N4-cyclohexyl-2-phenyl-N6-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 192631-88-2 CAPLUS CN 4,5,6-Pyrimidinetriamine, N4-butyl-2-phenyl-N6-(phenylmethyl)-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 192631-89-3 CAPLUS
CN 4,5,6-Pyrimidinetriamine, N4-pentyl-2-phenyl-N6-(phenylmethyl)-,
monohydrochloride (9CI) (CA INDEX NAME)

Me- (CH₂)
$$_4$$
-NH NH-CH₂-Ph

● HCl

$$Ph$$
 N
 N
 N
 $NH-CH_2-Ph$
 NH_2

● HCl

IT 192631-70-2P 192631-77-9P 192631-78-0P 192631-79-1P 192631-80-4P 192631-81-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 4,6-disubstituted and 4,5,6-trisubstituted 2-phenylpyrimidines and their Al adenosine receptor affinity)

RN 192631-70-2 CAPLUS

CN 4-Pyrimidinamine, 6-chloro-2-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 192631-77-9 CAPLUS

CN 4,6-Pyrimidinediamine, 5-nitro-2-phenyl-N,N'-bis(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 192631-78-0 CAPLUS

CN 4,6-Pyrimidinediamine, N-cyclopentyl-5-nitro-2-phenyl-N'-(phenylmethyl)(9CI) (CA INDEX NAME)

RN 192631-79-1 CAPLUS CN 4,6-Pyrimidinediamine, N-cyclohexyl-5-nitro-2-phenyl-N'-(phenylmethyl)-(9CI) (CA INDEX NAME)

RN 192631-80-4 CAPLUS

CN 4,6-Pyrimidinediamine, N-butyl-5-nitro-2-phenyl-N'-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 192631-81-5 CAPLUS

CN 4,6-Pyrimidinediamine, 5-nitro-N-pentyl-2-phenyl-N'-(phenylmethyl)- (9CI) (CA INDEX NAME)

Me- (CH₂)
$$_4$$
 - NH NO₂ NH- CH₂- Ph

IT 192631-76-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of 4,6-disubstituted and 4,5,6-trisubstituted 2-phenylpyrimidines and their Al adenosine receptor affinity) 192631-76-8 CAPLUS

4-Pyrimidinamine, 6-chloro-5-nitro-2-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN

CN

10/671,070

L10 ANSWER 88 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1997:151137 CAPLUS

DN 126:251130

TI A novel and efficient approach for the combinatorial synthesis of structurally diverse pyrimidines on solid support

AU Obrecht, Daniel; Abrecht, Christine; Grieder, Alfred; Villalgordo, Jose M.

CS Hoffmann-La Roche A.-G., Basel, CH-4070, Switz.

SO Helvetica Chimica Acta (1997), 80(1), 65-72 CODEN: HCACAV; ISSN: 0018-019X

PB Verlag Helvetica Chimica Acta

DT Journal

LA English

OS CASREACT 126:251130

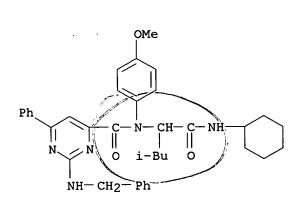
A versatile approach for the synthesis of 2,4,6-trisubstituted pyrimidines AB on solid support is described. Thus, polymer-bound thiouronium chloride reacted in high yield in a cyclocondensation reaction with RCOC.tplbond.CCO2CMe3 {R = Ph, 2-furyl, 5-benzo[1,3]dioxolyl} to form, after ester cleavage, polymer-bound pyrimidinecarboxylates which were cleaved by oxidation with MCPBA and pyrrolidine to give 85-90% pyrrolidinylpyrimidinecarboxylates I (R1 = OH) in 96-99% purities. Alternatively, Ugi 4-component condensation gave Ugi products such as I [R = Ph; R1 = NR2C(CHMe2)CONHR3; R2 = 4-MeOC6H4, Pr, cyclohexyl; R3 = cyclohexyl] in 65-87% yields. Multi-directional cleavage reaction of polymer-bound sulfone II with different nucleophiles resulted in the clean formation of pyrimidine-4-carboxamides. This strategy combines efficiently solid-phase chemical which a multicomponent reaction and a multi-directional cleavage step to form highly diverse pyrimidines in a parallel array.

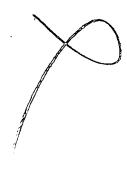
IT 188633-61-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (combinatorial synthesis of pyrimidines on solid support)

RN 188633-61-6 CAPLUS

CN 4-Pyrimidinecarboxamide, N-[1-[(cyclohexylamino)carbonyl]-3-methylbutyl]-N-(4-methoxyphenyl)-6-phenyl-2-[(phenylmethyl)amino]-(9CI) (CA INDEX NAME)





L10 ANSWER 89 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1997:26297 CAPLUS

DN 126:89387

TI Preparation of 5-[phenyl(methyl)- and pyridyl(methyl)]pyrimidine derivatives as pesticides

IN Kasahara, Isamu; Oooka, Hirohito; Murahashi, Kazuhiko; Matsuda, Mitsuhiko; Sano, Chikaaki

PA Nippon Soda Co, Japan

SO Jpn. Kokai Tokkyo Koho, 42 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.		DATE APPLICATION NO.		DATE	
PI	JP 08283246	A2	19961029	JP 1995-153806	19950529	
PRAI	JP 1994-142513	Α	19940601			
	JP 1995-51827	Α	19950216			

OS MARPAT 126:89387

AB The title compds. [I; Ar = (un)substituted Ph or pyridyl; n = 0.1; n = 0.1; R1 = H, halo, lower alkyl; R2 = H, lower alkyl or alkylthio; X = NR4, O, S; R3 = (CHR5)m-A1, (CHR6)k-O-A2, C1-12 alkyl, C2-12 alkenyl; m, k, = 1,2; wherein A1, A2 = (un)substituted Ph or pyridyl; R4 = H, lower alkyl or alkoxy; R5, R6 = H, lower alkyl], which are useful as agrochem. fungicides, insecticides, and aphicides, are prepared Thus, 0.4 g 4-chloro-5-phenylpyrimidine was dissolved in DMSO, treated with 0.42 g 2-(2,4-dimethylphenoxy)ethylamine and 0.3 g Et3N, and the resulting mixture was stirred at room temperature at 70° for 5 h to give 0.55 g of the title compound (II). II killed ≥80% Aphis gossypii on cucumber seedlings and Nilaparvata lugens on rice seedlings at 125 ppm and ≥80% Erysiphe graminis f.sp. tritici on wheat seedlings at 200 ppm.

IT 185052-66-8P 185052-68-0P 185052-71-5P 185052-72-6P 185052-74-8P 185052-75-9P 185052-76-0P 185052-78-2P 185052-79-3P 185052-80-6P 185052-81-7P 185052-83-9P 185052-87-3P 185052-91-9P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of [phenyl(methyl) - and pyridyl(methyl)]pyrimidine derivs. as pesticides)

RN 185052-66-8 CAPLUS

CN 4-Pyrimidinamine, 5-phenyl-N-(2-phenylethyl)- (9CI) (CA INDEX NAME)

RN 185052-68-0 CAPLUS

CN 4-Pyrimidinamine, 5-phenyl-N-[2-[2-(trifluoromethyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

RN 185052-71-5 CAPLUS

CN 4-Pyrimidinamine, 5-(2,4-dichlorophenyl)-N-(2-phenylethyl)- (9CI) (CA INDEX NAME)

RN 185052-72-6 CAPLUS

CN 4-Pyrimidinamine, 5-(2,4-dichlorophenyl)-N-[2-[2-(trifluoromethyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

RN 185052-74-8 CAPLUS

CN 4-Pyrimidinamine, 5-phenyl-N-[[3-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 185052-75-9 CAPLUS

CN 4-Pyrimidinamine, 5-(2,4-dichlorophenyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 185052-76-0 CAPLUS
CN 4-Pyrimidinamine, 5-(2,4-dichlorophenyl)-N-[[3-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 185052-78-2 CAPLUS
CN 4-Pyrimidinamine, 5-(4-methoxyphenyl)-N-(2-phenylethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N & NH-CH_2-CH_2-Ph \\ \hline \\ N & OMe \end{array}$$

RN 185052-79-3 CAPLUS
CN 4-Pyrimidinamine, 5-(4-methoxyphenyl)-N-[2-[2-(trifluoromethyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

RN 185052-80-6 CAPLUS

CN 4-Pyrimidinamine, 5-(4-methoxyphenyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 185052-81-7 CAPLUS

CN 4-Pyrimidinamine, 5-(4-methoxyphenyl)-N-[[3-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 185052-83-9 CAPLUS

CN 4-Pyrimidinamine, 6-chloro-5-phenyl-N-(2-phenylethyl)- (9CI) (CA INDEX NAME)

RN 185052-87-3 CAPLUS

CN 4-Pyrimidinamine, N-[(4-chlorophenyl)methyl]-N-ethoxy-5-phenyl- (9CI) (CA

INDEX NAME)

RN 185052-91-9 CAPLUS

CN 4-Pyrimidinamine, N-ethoxy-5-phenyl-N-(2-phenylethyl)- (9CI) (CA INDEX NAME)

10/671,070

L10 ANSWER 90 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1996:488269 CAPLUS

DN 125:211838

TI Electron-topological study of structure-activity relationship in the series of dihydrofolate reductase inhibitors

AU Vlasenko, S. P.; Dimoglo, A. S.

CS Inst. Chem., Acad. Sci. Moldova, Chisinau, Moldova

SO Khimiko-Farmatsevticheskii Zhurnal (1996), 30(6), 25-28 CODEN: KHFZAN; ISSN: 0023-1134

PB Izdatel'stvo Folium

DT Journal

LA Russian

AB An electron-topol. method for forecasting the inhibitory activity of 2-aminopyrimidine derivs. toward dihydrofolate reductase was developed. The parts of the mol. structure responsible for the binding to dihydrofolate reductase active site and hence for the inhibitory activity of the compds. were established.

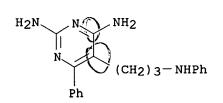
IT 2211-01-0

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(electron-topol. modeling of MSBAR of aminopyrimidines as dihydrofolate reductase inhibitors)

RN 2211-01-0 CAPLUS

CN 2,4-Pyrimidinediamine, 6-phenyl-5-[3-(phenylamino)propyl]- (9CI) (CA INDEX NAME)





L10 ANSWER 91 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1996:411057 CAPLUS

DN 125:114708

TI 4-Aminopyrimidine derivatives

IN Lee, Sung J.; Konishi, Yoshitaka; Macina, Orest T.; Kondo, Kigen; Yu, Dingwei T.; Miskowski, Tamara A.

PA Ono Pharmaceutical Co., Ltd., Japan

SO U.S., 28 pp., Cont.-in-part of U.S. Ser. No. 111,906, abandoned. CODEN: USXXAM

DT Patent

LA English

FAN.CNT 2

1741.0	PATENT NO.		DATE	APPLICATION NO.	DATE	
		KIND				
ΡI	US 5525604	Α	19960611	US 1994-295377	19940824	
	AT 163647	E	19980315	AT 1994-305973	19940812	
	ES 2114662	Т3	19980601	ES 1994-305973	19940812	
	JP 07089958	A2	19950404	JP 1994-222654	19940824	
	CA 2130878	AA	19950227	CA 1994-2130878	19940825	
	CA 2130878	С	19990323			
	CN 1109055	Α	19950927	CN 1994-109363	19940825	
	KR 204433	B1	19990615	KR 1994-21017	19940825	
PRAI	US 1993-111906	В2	19930826			

OS MARPAT 125:114708

AB 4-Aminopyrimidines I [A = bond, alkylene, oxyalkylene; Y = bond, alkylene, alkyleneoxy, alkoxyphenylene, phenylalkylene; Z = bond, CH:CH; R1 = heterocyclic containing 1 or 2 N atom; R2 = heterocyclic containing 1 or 2 N,

1 or

2 O or 1 S atom, carbocyclic, alkoxy, hydroxy alkoxy, OH; R3 = heterocyclic containing 1 or 2 N, 1 O, 1 S, or 1 N and 1 S atom, carbocyclic, halovinyl, H; n = 1, 2] with some exceptions, and acid addition salts thereof, inhibit cGMP-PDE, or TXA2 synthetase. Thus, 5-(3-methoxybenzyl)tetrahydro-2,4-pyrimidinedione was chlorinated, treated with H2NCH2CH2OCH2CH2OH and then imidazole to give the pyrimidine II, which had an IC50 against cGMP-PDE of 21.0 μM .

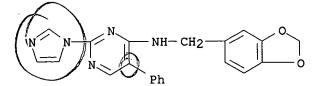
IT 163345-82-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 4-aminopyrimidine derivs. as cGMP phosphodiesterase and TXA2 synthase inhibitors)

RN 163345-82-2 CAPLUS

CN 4-Pyrimidinamine, N-(1,3-benzodioxol-5-ylmethyl)-2-(1H-imidazol-1-yl)-5phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

IT 163345-83-3P 163345-84-4P 163345-89-9P 163345-92-4P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 4-aminopyrimidine derivs. as cGMP phosphodiesterase and TXA2 synthase inhibitors)

RN 163345-83-3 CAPLUS

CN 4-Pyrimidinamine, N-(1,3-benzodioxol-5-ylmethyl)-2-(1H-imidazol-1-yl)-5-(4-methylphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

$$N \longrightarrow N \longrightarrow NH-CH_2 \longrightarrow O$$

$$Me$$

HCl

RN 163345-84-4 CAPLUS

CN 4-Pyrimidinamine, N-(1,3-benzodioxol-5-ylmethyl)-2-(1H-imidazol-1-yl)-5-(4-methoxyphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 163345-89-9 CAPLUS

CN 4-Pyrimidinamine, N-(1,3-benzodioxol-5-ylmethyl)-5-(4-chlorophenyl)-2-(1H-imidazol-1-yl)-, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 163345-92-4 CAPLUS

CN 4-Pyrimidinamine, N-(1,3-benzodioxol-5-ylmethyl)-2-(1H-imidazol-1-yl)-5-(2-naphthalenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

L10 ANSWER 92 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1996:184015 CAPLUS

DN 124:232480

TI Preparation and formulation of pyrimidine derivatives for treatment of kidney diseases

IN Yanaka, Mikiro; Nishijima, Fuyuhiko; Enari, Hiroyuki; Ise, Michihito

PA Kureha Chemical Industry Co., Ltd., Japan

SO Eur. Pat. Appl., 24 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

	PATENT NO.			KIND DATE		API	APPLICATION NO.		DATE	
D.T.					10051010		1005 10000			X
ΡI	EP 686631			A1	19951213	EP	1995-108380	19	9950601	
	EP 686631			В1	20010117					/
		T, BE,	CH,	DE,	DK, FR, GB,	IT, L	, NL	*	/	
	CA 215060	9		AA	19951202	CA	1995-2150609	9 19	9950531/	
	CA 215060	9		С	19981208				ij	
	US 558538	1		Α	19961217	US	1995-454629	19	9950531	
	AU 952042	7		A 1	19960104	AU	1995-20427	19	9950601	
	AU 679361			В2	19970626					
	JP 080486	72		A2	19960220	JP	1995-158658	19	9950601	
	JP 299660	9		В2	20000111					
	AT 198746			E	20010215	AT	1995-108380	19	9950601	
PRAI	JP 1994-1	42274		Α	19940601					
os	MARPAT 12	4:2324	80							

AB The title compds. I [R1 = H, alkyl, etc.; R2 = H, halo, etc.; R3 = CO2H, etc.] are claimed. In rats (with exptl. kidney disease) dosed with I [R1 = butyl; R2 = 6-Cl; R3 = 4-CO2Me] (preparation given) at 20 mg/kg/day, the survival time was 6.9 wk, vs. 5 wk in untreated controls, and 6.9 wk in rats treated with DuP753. The title compds. do not show angiotensin II receptor antagonism.

IT 174697-58-6P 174697-83-7P 174697-86-0P 174697-87-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrimidine derivs. for treatment of kidney diseases)

RN 174697-58-6 CAPLUS

CN Benzoic acid, 4-[[[5-[(1-oxopentyl)amino]-6-phenyl-4-pyrimidinyl]amino]methyl]- (9CI) (CA INDEX NAME)

RN 174697-83-7 CAPLUS

CN Pentanamide, N-[4-[[(4-hydroxyphenyl)methyl]amino]-6-phenyl-5-pyrimidinyl](9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \text{OH} \\ & & & \\ \text{Ph} & & & \\ & & & \\ \text{N-Bu-C-NH} & & \\ & & & \\ & & & \\ & & & \\ \end{array}$$

RN

174697-86-0 CAPLUS
Pentanamide, N-[4-[[[4-(methylamino)phenyl]methyl]amino]-6-phenyl-5-CN pyrimidinyl] - (9CI) (CA INDEX NAME)

174697-87-1 CAPLUS RN

Pentanamide, N-[4-[[[4-(dimethylamino)phenyl]methyl]amino]-6-phenyl-5-CN pyrimidinyl] - (9CI) (CA INDEX NAME)

- L10 ANSWER 93 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
- 1995:573846 CAPLUS AN
- DN 122:314567
- Preparation of 4-aminopyrimidine cyclic-guanosine monophosphate-ΤI phosphodiesterase and thromboxane A2 synthetase inhibitors
- Lee, Sung Jai; Konishi, Yoshitaka; Macina, Orest Taras; Kondo, Kigen; Yu, IN Dingwei Tim; Miskowski, Tamara Ann
- Ono Pharmaceutical Co., Ltd., Japan PA
- SO Eur. Pat. Appl., 56 pp. CODEN: EPXXDW
- DTPatent
- LΑ English
- ביאאו ראויי 2

PAN.	UNI Z				\ /
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PΙ	EP 640599	A1	19950301	EP 1994-305973	19940812
	EP 640599	B1	19980304		
	R: AT, BE, CH,	DE, DK	, ES, FR, GB	, GR, IE, IT, LI, LU,	MC, NL, PT, SE
	AT 163647	E	19980315	AT 1994-305973	19940812
	ES 2114662	Т3	19980601	ES 1994-305973	19940812
	JP 07089958	A2	19950404	JP 1994-222654	19940824
	CA 2130878	AA	19950227	CA 1994-2130878	19940825
	CA 2130878	С	19990323		
	CN 1109055	Α	19950927	CN 1994-109363	19940825
	KR 204433	B1	19990615	KR 1994-21017	19940825
PRAI	US 1993-111906	Α	19930826		
Oς	MARPAT 122:314567				

MARPAT 122:314567

The title compds. [I; A = direct bond, C1-4 alkylene or oxyalkylene; R1 = AB 4-15-membered (un) substituted heterocyclyl; R2= 4-15-membered (un) substituted heterocyclyl, C4-15 carbocyclyl, C1-4 alkoxy, hydroxyalkoxy, OH; R3 = 4-15-membered (un) substituted heterocyclyl, C4-15 carbocyclyl, SONR7R8, H, etc.; R7, R8 = H, alkyl; Y = direct bond, C1-4 alkylene, alkyleneoxy, alkoxyphenylene, phenylalkylene; Z = direct bond, vinylene; 1 = 1, 2], which are inhibitors of cGMP-PDE and TXA2 synthetase, useful for the treatment of hypertension (no data), peptic ulcer (no data), etc., are prepared and a I-containing formulation presented. Thus, aminopyrimidine II (m.p. 153.0-156.0°) was prepared and demonstrated 100% inhibition of TXA2 synthetase at 10 µM.

IT 163345-40-2P 163345-41-3P 163345-47-9P 163345-50-4P

RL: PNU (Preparation, unclassified); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(claimed compound; preparation of 4-aminopyrimidine cyclic-guanosine monophosphate-phosphodiesterase and thromboxane A2 synthetase inhibitors)

RN 163345-40-2 CAPLUS

4-Pyrimidinamine, N-(1,3-benzodioxol-5-ylmethyl)-2-(1H-imidazol-1-yl)-5-(4-CN methylphenyl) - (9CI) (CA INDEX NAME)

RN 163345-41-3 CAPLUS

CN 4-Pyrimidinamine, N-(1,3-benzodioxol-5-ylmethyl)-2-(1H-imidazol-1-yl)-5-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

RN 163345-47-9 CAPLUS

CN 4-Pyrimidinamine, N-(1,3-benzodioxol-5-ylmethyl)-5-(4-chlorophenyl)-2-(1H-imidazol-1-yl)- (9CI) (CA INDEX NAME)

RN 163345-50-4 CAPLUS

CN 4-Pyrimidinamine, N-(1,3-benzodioxol-5-ylmethyl)-2-(1H-imidazol-1-yl)-5-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

IT 163345-82-2P 163345-83-3P 163345-84-4P 163345-89-9P 163345-92-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 4-aminopyrimidine cyclic-guanosine monophosphatephosphodiesterase and thromboxane A2 synthetase inhibitors)

RN 163345-82-2 CAPLUS

CN 4-Pyrimidinamine, N-(1,3-benzodioxol-5-ylmethyl)-2-(1H-imidazol-1-yl)-5-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

$$N \longrightarrow N \longrightarrow N \to N \to CH_2 \longrightarrow O$$

HCl

RN 163345-83-3 CAPLUS

CN 4-Pyrimidinamine, N-(1,3-benzodioxol-5-ylmethyl)-2-(1H-imidazol-1-yl)-5-(4-methylphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} N & N & NH-CH_2 \\ \hline & N & \\ & & \\$$

● HCl

RN 163345-84-4 CAPLUS

CN 4-Pyrimidinamine, N-(1,3-benzodioxol-5-ylmethyl)-2-(1H-imidazol-1-yl)-5-(4-methoxyphenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 163345-89-9 CAPLUS

CN 4-Pyrimidinamine, N-(1,3-benzodioxol-5-ylmethyl)-5-(4-chlorophenyl)-2-(1H-imidazol-1-yl)-, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 163345-92-4 CAPLUS

CN 4-Pyrimidinamine, N-(1,3-benzodioxol-5-ylmethyl)-2-(1H-imidazol-1-yl)-5-(2-naphthalenyl)-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

L10 ANSWER 94 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1995:542200 CAPLUS

DN 123:83308

TI Synthesis of functionalized pyrimidine-4-thiones and pyrido[2,3-d]pyrimidin-5-one derivatives from aminals of monoacylketenes

AU Dorokhov, V. A.; Komkov, A. V.; Shashkova, E. M.; Bogdanov, V. S.; Bochkareva, M. N.

CS N. D. Zelinsky Inst. Org. Chem., Russian Acad. Sci., Moscow, 117913, Russia

SO Izvestiya Akademii Nauk, Seriya Khimicheskaya (1993), (11), 1932-7 CODEN: IASKEA

PB Institut Organicheskoi Khimii im. N. D. Zelinskogo Rossiiskoi Akademii Nauk

DT Journal

LA Russian

AB Monoacylketene aminals containing an unsubstituted NH2 group react with benzoyl isothiocyanate as C-nucleophiles yielding the corresponding thioamides, which are cyclized by sodium methoxide in methanol to 6-amino-5-acetyl-2-phenyl-4(3H)-pyrimidinethiones, e.g., I.. Reaction of the thiones with DMF di-Me acetal leads to 4-(methylthio)pyrido[2,3-d]pyrimidin-5(8H)-ones, e.g., II (R = H, R1 = Ph). Cyclization of 5-acetyl-6-benzamido-4-(methylthio)-2-phenylpyrimidine by sodium methoxide yields II (R = Ph, R1 = H).

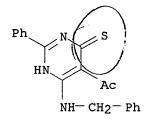
IT 165401-59-2P 165401-65-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(functionalized pyrimidinethiones and pyridopyrimidinones from acylketene aminals)

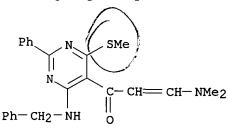
RN 165401-59-2 CAPLUS

CN Ethanone, 1-[1,4-dihydro-2-phenyl-6-[(phenylmethyl)amino]-4-thioxo-5-pyrimidinyl]- (9CI) (CA INDEX NAME)



RN 165401-65-0 CAPLUS

CN 2-Propen-1-one, 3-(dimethylamino)-1-[4-(methylthio)-2-phenyl-6-[(phenylmethyl)amino]-5-pyrimidinyl]- (9CI) (CA INDEX NAME)



L10 ANSWER 95 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1995:484203 CAPLUS

DN 123:55795

TI Synthesis and immunomodulatory activity of 6-methyl-2-phenyl-5-substituted pyrimidines

AU Cieplik, Jerzy; Machon, Zdzislaw; Zimecki, Michal; Wieczorek, Zbigniew

CS Dep. Org. Chemistry, Medical Academy, Wroclaw, 50-137, Pol.

SO Farmaco (1995), 50(2), 131-6

CODEN: FRMCE8

PB Societa Chimica Italiana

DT Journal

LA English

AB Various new 4-arylamino-6-methyl-2-phenyl-5-methylamino- and 5-alkoxymethylpyrimidines were synthesized in two chemical series from 4-arylamino-6-methyl-2-phenyl-5-hydroxymethylpyrimidines. Some of these products display immunomodulatory activities comparable to that of levamisole.

IT 164927-01-9P 164927-02-0P 164927-06-4P 164927-07-5P 164927-08-6P 164927-09-7P 164927-10-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(synthesis and immunomodulatory activity of substituted pyrimidines)

RN 164927-01-9 CAPLUS

CN 5-Pyrimidinemethanamine, 4-[(4-chlorophenyl)amino]-N-(4-ethoxyphenyl)-6-methyl-2-phenyl- (9CI) (CA INDEX NAME)



RN 164927-02-0 CAPLUS

CN 5-Pyrimidinemethanamine, N-(4-chlorophenyl)-4-[(4-chlorophenyl)amino]-6-methyl-2-phenyl- (9CI) (CA INDEX NAME)

RN 164927-06-4 CAPLUS

CN 5-Pyrimidinemethanamine, 4-[(4-chlorophenyl)amino]-N-(2,6-dichlorophenyl)-6-methyl-2-phenyl-(9CI) (CA INDEX NAME)

RN 164927-07-5 CAPLUS

CN 5-Pyrimidinemethanamine, N-(4-ethoxyphenyl)-4-methyl-2-phenyl-6-(phenylamino)- (9CI) (CA INDEX NAME)

RN 164927-08-6 CAPLUS

CN 5-Pyrimidinemethanamine, N-(4-chlorophenyl)-4-methyl-2-phenyl-6-(phenylamino)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Ph} & \text{Me} & \text{C1} \\ & \text{N} & \text{CH}_2 - \text{NH} \end{array}$$

RN 164927-09-7 CAPLUS

CN 5-Pyrimidinemethanamine, N-(4-chlorophenyl)-4-[(4-ethoxyphenyl)amino]-6-methyl-2-phenyl- (9CI) (CA INDEX NAME)

RN 164927-10-0 CAPLUS

CN 5-Pyrimidinemethanamine, N-(4-ethoxyphenyl)-4-[(4-ethoxyphenyl)amino]-6-methyl-2-phenyl- (9CI) (CA INDEX NAME)

L10 ANSWER 96 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1994:605382 CAPLUS

DN 121:205382

TI Aminopyrimidine derivatives and their production and use.

IN Ohtsuka, Toshikazu; Masui, Moriyasu; Takeda, Takami; Masuko, Michio; Ohba, Katsuaki

PA Shionogi and Co., Ltd., Japan

SO Eur. Pat. Appl., 85 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

ran.		ENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI		506011	A1	19940713	EP 1993-310556	19931224
			•		GB, GR, IE, IT, LI,	
		5439911 L49491	A E	19950808 19970315	US 1993-168217 AT 1993-310556	19931217 19931224
		2101254	T3	19970701		19931224
		06279417 3366715	A2 B2	19941004 20030114	JP 1993-353743	19931227
		5519139	A	19960521	US 1995-448193	19950523
PRAI		1992-348535 1993-14980	A A	19921228 19930201		
	US 1	1993-168217	A3	19931217		

OS MARPAT 121:205382

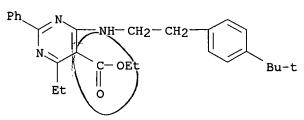
AB The title compds., i.e. 4-amino-5-pyrimidinecarboxylates I (R1 = H, halo, alkyl, etc.; R2 = alkyl; R3 = H, alkyl, alkenyl, etc.; R4 = H, alkyl; R5, R6, R11 = H, halo, alkyl, alkoxy, etc.; X = alkanediyl, alkyleneoxy) were disclosed. I were claimed as fungicides, insecticides and miticides. A specifically claimed example compound is Et 4-[[2-[4-(difluoromethoxy)phenyl]ethyl]amino]-6-ethyl-5-pyrimidinecarboxylate (II).

IT 157980-55-7P 157981-15-2P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as insecticide, fungicide or miticide)

RN 157980-55-7 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[2-[4-(1,1-dimethylethyl)phenyl]ethyl]amin o]-6-ethyl-2-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 157981-15-2 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-6-ethyl-2-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

L10 ANSWER 97 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1994:217513 CAPLUS

DN 120:217513

TI Synthesis of [1,5-a]pyrimidinone ring derivatives

AU Rashed, N.; Mousaad, A.; Saleh, A.

CS Fac. Sci., Alexandria Univ., Alexandria, Egypt

SO Journal of the Chinese Chemical Society (Taipei, Taiwan) (1993), 40(4), 393-7
CODEN: JCCTAC; ISSN: 0009-4536

DT Journal

LA English

AB Cyclodehydrogenation of the benzalhydrazino derivs. I (Ar = 4-MeOC6H4, R = H, Me) gave 6-cyano-7-(4-methoxyphenyl)-2-phenyl-5-oxo-1,2,4-triazolo[1,5-a]pyrimidine (II) and 6-cyano-7-(4-methoxyphenyl)-4-methyl-2-phenyl-5-oxo-1,2,4-triazolo[1,5-a]pyrimidine (III), resp. Methylation, acetylation and benzylation of I (R = H) gave the corresponding N-Me, acetyl and benzyl derivs. Acetylation of I (R = H) with boiling acetic anhydride afforded the diacetyl derivative IV; its benzylation gave the mono-N-benzyl derivative

IT 153896-60-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 153896-60-7 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(4-methoxyphenyl)-4-oxo-2-[(phenylmethyl) (phenylmethylene)hydrazino]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} Ph-CH=N \\ Ph-CH_2-N & H \\ N & O \end{array}$$



L10 ANSWER 98 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1994:4377 CAPLUS

DN 120:4377

- TI Identification of highly potent and selective inhibitors of Toxoplasma gondii dihydrofolate reductase
- AU Chio, Li Chun; Queener, Sherry F.
- CS Sch. Med., Indiana Univ., Indianapolis, IN, 46202-5120, USA
- SO Antimicrobial Agents and Chemotherapy (1993), 37(9), 1914-23 CODEN: AMACCQ; ISSN: 0066-4804
- DT Journal
- LA English
- AΒ Toxoplasma gondii RH was obtained in high yield from culture in RPMI medium on a line of Chinese hamster ovary cells lacking dihydrofolate reductase activity (ATCC 3952 dhfr-). Dihydrofolate reductase prepns. from harvested organisms had sp. activities of 22.9 nmol/min/mg. The 50% inhibitory concns. against reference compds. were 0.014 µM for methotrexate, 0.25 μM for pyrimethamine, 2.7 μM for trimethoprim, and 0.010 μM for trimetrexate. The Km value for NADPH was 11 μM and followed Michaelis-Menten kinetics; the Km for dihydrofolate was .apprx.11 μΜ, but substrate inhibition appeared to occur at high substrate concns. Dihydrofolate reductase from T. gondii was used to screen 130 compds. from the National Cancer Institute repository. Thirteen compds. were >100-fold more potent than pyrimethamine toward T. gondii dihydrofolate reductase; 6 compds. with various potencies were 8-46 times as selective as pyrimethamine for the protozoal form of the enzyme over the mammalian Four trimetrexate analogs were more potent than trimetrexate, and 2 were significantly more selective. Representative compds. were also tested in a culture model of T. gondii employing uracil incorporation as an index of growth. One pyrimethamine analog was as effective as pyrimethamine in inhibiting T. gondii in culture (50% inhibitory concentration, $0.45~\mu M)$. Three other compds. were also effective at micromolar concns.
- IT 136242-86-9

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(dihydrofolate reductase of Toxoplasma gondii inhibition by, structure in relation to)

RN 136242-86-9 CAPLUS

CN 2,4-Pyrimidinediamine, 5-(4-chlorophenyl)-6-[[(4-nitrophenyl)amino]methyl]-(9CI) (CA INDEX NAME)



L10 ANSWER 99 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1993:671185 CAPLUS

DN 119:271185

TI Heterocyclic 4-pyrimidinamine derivatives

IN Edwards, Martin Paul; Ratcliffe, Arnold Harry

PA Imperial Chemical Industries PLC, UK

SO Ger. Offen., 29 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

r A	ran.cni i							
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE			
PI	DE 4239440	A 1	19930609	DE 1992-4239440	19921124			
	CA 2082668	AA	19930605	CA 1992-2082668	19921112			
	ZA 9208742	Α	19930609	ZA 1992-8742	19921112			
	FR 2684672	A1	19930611	FR 1992-14376	19921130			
	NL 9202091	A	19930701	NL 1992-2091	19921202			
	GB 2262096	A1	19930609	GB 1992-25283	19921203			
	BE 1005473	A 3	19930803	BE 1992-1065	19921203			
	JP 05255327	A 2	19931005	JP 1992-325478	19921204			
PR	AI GB 1991-25842	Α	19911204					

OS MARPAT 119:271185

AB The title compds., 4-pyrimidinamine derivs. are claimed. These compds. are potentially useful for as antihypertensives and the treatment of congestive heart failure. Thus, 2,6-dimethyl-N-[[2'-(1H-tetrazol-5-yl)biphenyl-4-yl]methyl]-4-pyrimidinamine hydrochloride (I) was prepared in several steps. I had activity as angiotensin II antagonist.

IT 150358-31-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 150358-31-9 CAPLUS

CN 4-Pyrimidinamine, 2,6-diethyl-5-(4-methylphenyl)-N-[[2'-[2-(triphenylmethyl)-2H-tetrazol-5-yl][1,1'-biphenyl]-4-yl]methyl]- (9CI) (CA INDEX NAME)



L10 ANSWER 100 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1992:633688 CAPLUS

DN 117:233688

TI Autorecycling oxidation of alcohols catalyzed by pyridodipyrimidines as an NAD(P) + model

AU Nagamatsu, Tomohisa; Yamato, Hirotake; Ono, Masami; Takarada, Shigeki; Yoneda, Fumio

CS Fac. Pharm. Sci., Okayama Univ., Okayama, 700, Japan

SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1992), (16), 2101-9 CODEN: JCPRB4; ISSN: 0300-922X

DT Journal

LA English

AB Pyridodipyrimidinetetrones I (R = H, Me, Ph; R1 = alkyl, Ph) have been synthesized by the condensation of 6-aminouracils with 6-chloro-5-formyluracils in DMF. Pyridodipyrimidinetriones II (R1 = alkyl, Ph; R2 = H, alkyl) have been synthesized by the condensation of 6-amino-2-phenylpyrimidin-4(3H)-ones with 2,4,6-trichloropyrimidine-5-carboxaldehyde in AcOH. I and II catalyze the oxidation of alcs. under neutral conditions (in the absence of base) to yield carbonyl compds., with a remarkably high turnover number The oxidation yields were markedly dependent upon the presence of lipophilic substituents, particularly of a longer alkyl group at the 10-position. These catalysts are so stable that the oxidation reaction proceeds until the substrate is exhausted.

IT 144486-32-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with formylpyridines)

RN 144486-32-8 CAPLUS

CN 4(1H)-Pyrimidinone, 2-phenyl-6-[(2-phenylethyl)amino]- (9CI) (CA INDEX NAME)

Ph
$$\stackrel{\text{H}}{\underset{\text{N}}{\bigvee}}$$
 NH- CH₂- CH₂- Ph



- L10 ANSWER 101 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1992:448462 CAPLUS
- DN 117:48462
- TI Reactivity of 6-anisyl-5-cyano-4-oxo-2-thioxo-1,2,3,4-tetrahydropyrimidine towards some electrophiles and nucleophiles
- AU Hassan, M. F. Madkour; Mahamed, A. E. Sayed; Ashraf, A. Hamed; Adel, M. Gaber; Abd El-Khalik, A. Hataba
- CS Fac. Sci., Ain Shams Univ., Cairo, Egypt
- SO Chinese Journal of Chemistry (1991), 9(3), 262-9 CODEN: CJOCEV; ISSN: 1001-604X
- DT Journal
- LA English
- AB The title compound I was subjected to reaction with some electrophiles and nucleophiles, such as alkyl halides, Et chloroacetate, or amines, hydrazines etc. The resulting compds. were used in further syntheses for the purpose of obtaining some new types of heterocycles with possible biol. and pharmaceutical activities.
- IT 138609-06-0P
 - RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
- RN 138609-06-0 CAPLUS
- CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-6-(4-methoxyphenyl)-4-oxo-2-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

L10 ANSWER 102 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1991:647448 CAPLUS

DN 115:247448

TI Pneumocystis carinii dihydrofolate reductase used to screen potential antipneumocystis drugs

AU Broughton, M. Christine; Queener, Sherry F.

CS Sch. Med., Indiana Univ., Indianapolis, IN, 46202-5120, USA

SO Antimicrobial Agents and Chemotherapy (1991), 35(7), 1348-55 CODEN: AMACCQ; ISSN: 0066-4804

DT Journal

LA English

P. carinii was obtained in high yield from the lungs of immunosuppressed AB rats by rupturing mammalian host cells, washing away the soluble mammalian dihydrofolate reductase, and harvesting intact organisms in association with the mammalian plasma membranes. P. carinii dihydrofolate reductase, measured in the 100,000 + g supernatant from sonicated organisms, was obtained in yields ranging up to 62 IU per rat. The enzyme prepared in the presence of protease inhibitors was stable when frozen in liquid nitrogen. P. carinii dihydrofolate reductase differed from the mammalian enzyme in that the former was slightly inhibited by 150 mM KCl, whereas the latter was stimulated over twofold by 150 mM KCl. The standard assay for P. carinii dihydrofolate reductase contained 0.12 mM NADPH and 92 μM dihydrofolic acid. Under these conditions, the 50% inhibitory concns. of the known inhibitors trimethoprim, trimetrexate, and pyrimethamine were 12 $\mu M,~42~nM,~and~3.8~\mu M,~resp.$ These standard compds. were also tested against dihydrofolate reductase from rat liver to allow an assessment of the selectivity of the drugs. Although it was the least potent, trimethoprim was the most selective. Pyrimethamine was more potent but was nonselective. Trimetrexate was extremely potent but was selective for mammalian dihydrofolate reductase. A series of exptl. compds. was obtained from the National Cancer Institute and other sources through the Developmental Therapeutics Branch of the Division of AIDS at the National Institute of Allergy and Infectious Diseases. Among the first 87 compds. tested, 11 had 50% inhibitory concns. below that of trimetrexate and 3 were more selective than trimethoprim. The most promising compds. in this original group were chemical related to methotrexate.

IT 136242-86-9

RL: BIOL (Biological study)

(dihydrofolate reductase from liver vs. Pneumocystis carinii inhibition by, AIDS therapy and mol. structure in relation to)

RN 136242-86-9 CAPLUS

CN 2,4-Pyrimidinediamine, 5-(4-chlorophenyl)-6-[[(4-nitrophenyl)amino]methyl]-(9CI) (CA INDEX NAME)

$$\begin{array}{c|c} H_2N & N & CH_2-NH \\ \hline & N & N & CH_2-NH \\ \hline & N & NO_2 \\ \hline & NH_2 & C1 \\ \end{array}$$



L10 ANSWER 103 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1991:57530 CAPLUS

DN 114:57530

TI 2-Iodopropargyloxypyrimidines and agrochemical microbicides containing them

IN Masuda, Katsumi; Ito, Shigehisa; Maeno, Shinichiro; Eguchi, Katsumi; Hasegawa, Keisuke

PA Kumiai Chemical Industry Co., Ltd., Japan; Ihara Chemical Industry Co., Ltd.

SO Jpn. Kokai Tokkyo Koho, 12 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

2.4., 4., 2						
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
ΡI	JP 02200678	A2	19900808	JP 1989-18778	19890128	
PRAJ	JP 1989-18778		19890128			

OS MARPAT 114:57530

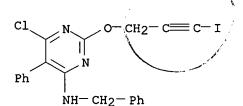
AB Agrochem. microbicides contain the title compds. I [R1 = H, halo, (halo)alkyl, alkoxy; R2 = H, halo, alkyl, alkoxy, alkylthio, Ph; R3 = H, alkyl; R4 = (alkoxy, cyclo, or alkoxycarbonyl)alkyl, alkenyl alkynyl, CR5R6C6H4X; R5, R6 = H, alkyl; X = H, halo, alkyl, alkoxy; R3R4 may form 5- or 6-membered heterocycle] as active ingredients. NaH in benzene was stirred with propargyl alc. at room temperature for 2.5 h and treated with 4-chloro-6-diethylamino-2-methylsulfonylpyrimidine at 6-15° for 1.5 h to give 99.2% 4-chloro-6-diethylamino-2-propargyloxypyrimidine, which was iodinated with NaOH and iodine in MeOH at room temperature for 2.5 h to afford 81.0% I (R1 = C1, R2 = H, R3 = R4 = Et) (II). II was applied to cucumber at 50 ppm to show ≥90% control of Pseudoperonospora cubensis after 7 days, vs. <40% control, for a conventional fungicide.

IT 130718-37-5P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as agrochem. microbicide)

RN 130718-37-5 CAPLUS

CN 4-Pyrimidinamine, 6-chloro-2-[(3-iodo-2-propynyl)oxy]-5-phenyl-N-(phenylmethyl)--(9CI) (CA INDEX NAME)





L10 ANSWER 104 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1989:515128 CAPLUS

DN 111:115128

TI Azolopyrimidines and pyrimidoquinazolines from 4-chloropyrimidines

AU El-Reedy, A. M.; Ali, A. S.; Ayyad, A. O.

CS Fac. Sci., Univ. Cairo, Giza, Egypt

SO Journal of Heterocyclic Chemistry (1989), 26(2), 313-16 CODEN: JHTCAD; ISSN: 0022-152X

DT Journal

LA English

OS CASREACT 111:115128

AB 5-Cyano-3,4-dihydro-6-phenyl-2-substituted pyrimidinones reacted with phosphorus oxychloride to give the corresponding 4-chloropyrimidine derivs. I (R = Ph, NHPh, NHCH2Ph, Rl = Cl). Compds. I (Rl = Cl) reacted with aniline and hydrazine to yield I (R = Ph, NHPh, NHCH2Ph; Rl = NHPh, NHNH2). The hydrazino derivs. could be converted into the triazolo- and tetrazolopyrimidines II (R2 = Ph, NHCH2Ph) and III by the action of CS2 and nitrous acid, resp. The reaction of I (R = NHPh, NHCH2Ph; Rl = Cl) with phenylhydrazine afforded directly the 5-amino-4,6-diphenyl-6H-2-substituted pyrazolopyrimidines IV (same R2). The 4-chloro derivative I (R = Ph, Rl = Cl) reacted with anthranilic acid to form the 5-cyano-2,4-diphenyl-6-(o-carboxyphenylamino)pyrimidine, which could be cyclized into the 4-cyano-1,3-diphenyl-10H-pyrimido[6,1-b]quinazolin-10-one by heating with acetic anhydride.

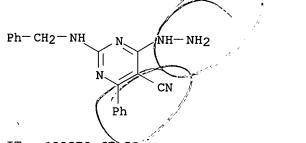
IT 122379-68-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclocondensation reaction of, with carbon disulfide)

RN 122379-68-4 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-hydrazino-6-phenyl-2-[(phenylmethyl)amino](9CI) (CA INDEX NAME)



IT 122379-67-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclocondensation reaction of, with phenylhydrazine, aminopyrazolopyrimidine from)

RN 122379-67-3 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-chloro-6-phenyl-2-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

IT 122379-65-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with phosphorus oxychloride, chloropyrimidine derivative from)

RN 122379-65-1 CAPLUS

CN 5-Pyrimidinecarbonitrile, 1,4-dihydro-4-oxo-6-phenyl-2-

[(phenylmethyl)amino] - (9CI) (CA INDEX NAME)

L10 ANSWER 105 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1989:95143 CAPLUS

DN 110:95143

TI Synthesis of pyrimidine derivatives by the reaction of ketene dithioacetals with amides

AU Kohra, Shinya; Tominaga, Yoshinori; Hosomi, Akira

CS Fac. Pharm. Sci., Nagasaki Univ., Nagasaki, 852, Japan

SO Journal of Heterocyclic Chemistry (1988), 25(3), 959-68 CODEN: JHTCAD; ISSN: 0022-152X

DT Journal

LA English

OS CASREACT 110:95143

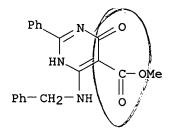
Reactions of Me 2-cyano-3,3-bis (methylthio) acrylate (MeS) 2C:CRCN (I, R = CO2Me) with carboxamides R1CONH2(II, R1 = 4-R2C6H4, C1CH2, Me, PhCH:CH; R2 = H, NO2, Me, MeO) in the presence of NaH gave the resp. Me 3-N-acylamino-2-cyano-3-(methylthio) acrylates R1CONaC(SMe):C(CO2Me)CN, which were readily converted to the resp. pyrimidine derivs. III (R = CO2Me) at reflux in methanol in good yields. Reactions of 2-cyano-3,3-bis (methylthio) acrylonitrile I (R = CN) with the carboxamides II gave directly pyrimidine-5-carbonitrile derivs. III (R = CN). Ketene dithioacetals smoothly reacted with thioacetamide or ureas to give the expected pyrimidine derivs. Polyfunctionalized pyrimidines, thus obtained, were also used for the synthesis of fused pyrimidine derivs.

IT 87694-01-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 87694-01-7 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,4-dihydro-4-oxo-2-phenyl-6-[(phenylmethyl)amino]-, methyl ester (9CI) (CA INDEX NAME)





L10 ANSWER 106 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1989:77445 CAPLUS

DN 110:77445

TI Light stabilizers for dyed polyester fibers

IN Reinert, Gerhard; Burdeska, Kurt

PA Ciba-Geigy A.-G., Switz.

SO Eur. Pat. Appl., 13 pp.

CODEN: EPXXDW

DT Patent

LA German

FAN.CNT 1

FAN.	CNT I				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 280654	A 1	19880831	EP 1988-810106	19880222
	EP 280654	B1	19920513		
	R: AT, BE, CH,	DE, ES	, FR, GB, IT	, LI, SE	
	AT 76131	E	19920515	AT 1988-810106	19880222
	ES 2032594	Т3	19930216	ES 1988-810106	19880222
	AU 8812325	A 1	19880901	AU 1988-12325	19880226
	AU 607188	B2	19910228		
	JP 63227879	A2	19880922	JP 1988-42448	19880226
	BR 8800824	Α	19881004	BR 1988-824	19880226
	ZA 8801376	Α	19881026	ZA 1988-1376	19880226
	US 4895981	Α	19900123	US 1989-331071	19890324
PRAI	CH 1987-751	Α	19870227		
	CH 1987-3820	Α	19871001		
	US 1988-156771	A1	19880217		
	EP 1988-810106	Α	19880222		
	440 55445				

OS MARPAT 110:77445

AB The pyrimidines I [R = alkyl, alkoxy, halogen, OH; R1 = alkyl; R2 = H, halogen, amino, alkoxy, alkenyl, Ph (optionally substituted); m = 0 or 1; n = 0-2] are light stabilizers for dyed polyester fibers which need not be incorporated in the fibers. A polyester fabric was dyed with a disperse dye in a dyebath containing 1.65% 6-(4-ethoxy-2-hydroxyphenyl-4-methyl-2-phenylpyrimidine (II), giving dyeings with Ford lightfastness 3-4, 3-4, and 3-4 after 0 and 1 h at 180° or 1 h at 200°, resp.; vs. 1-2, 1-2, and 1-2, resp., without II, and 3-4, 3-4, and 2-3, resp., with a benzotriazole in place of II.

IT 118823-24-8

RL: USES (Uses)

(light stabilizers, for dyed polyester fibers)

RN 118823-24-8 CAPLUS

CN Phenol, 5-ethoxy-2-[2-phenyl-6-[(2-phenylethyl)amino]-4-pyrimidinyl]-(9CI) (CA INDEX NAME)



L10 ANSWER 107 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1988:406537 CAPLUS

DN 109:6537

TI New 2-substituted amino-6-(2-hydroxyphenyl)pyrimidine derivatives as blood platelet aggregation inhibitors and a process for preparing them

IN Murakami, Yukitoshi; Takagi, Kaname

PA Zeria Pharmaceutical Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 10 pp. CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 62255487	A2	19871107	JP 1986-97991	19860430
PRAI	JP 1986-97991		19860430		

OS CASREACT 109:6537

AB The title compds. (I; R1 = lower alkylamino, lower dialkylamino, cyclic amino, aralkylamino; R2 = O2N, NH2) (II), useful as blood platelet aggregation inhibitors, were prepared A solution of 5 mmol I (R1 = SMe, R2 = O2N) and 50% aqueous cyclohexylamine was refluxed 2 h to give 98.5% I (R1 = cyclohexylamino, R2 = O2N) which was hydrogenated over 5% Pd/C to give, after acidification with 2N aqueous HCl, I (R1 = cyclohexylamino, R2 = NH2).HCl (III). III inhibited collagen-induced blood platelet aggregation with a IC50 of 39.8 µM in platelet rich plasma of a dog.

IT 114798-05-9P 114798-06-0P 114798-21-9P 114798-22-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as blood platelet aggregation inhibitor)

RN 114798-05-9 CAPLUS

CN Phenol, 2-[6-methyl-5-nitro-2-[(phenylmethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

RN 114798-06-0 CAPLUS

CN Phenol, 2-[6-methyl-5-nitro-2-[(2-phenylethyl)amino]-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$Ph-CH_2-CH_2-NH$$
 N
 NO_2
 Me

RN 114798-21-9 CAPLUS

CN Phenol, 2-[5-amino-6-methyl-2-[(phenylmethyl)amino]-4-pyrimidinyl]-, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 114798-22-0 CAPLUS

CN Phenol, 2-[5-amino-6-methyl-2-[(2-phenylethyl)amino]-4-pyrimidinyl]-, monohydrochloride (9CI) (CA INDEX NAME)

$$Ph-CH_2-CH_2-NH$$
 N
 NH_2
 Me

HCl

L10 ANSWER 108 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1988:150408 CAPLUS

DN 108:150408

TI Syntheses of 2,3-dihydro-5H-thiazolo[3,2-a]pyrimidines and tetrasubstituted dihydropyrimidine derivatives as possible anthelmintic agents

AU Akhtar, M. Shamim; Seth, M.; Bhaduri, A. P.

CS Div. Med. Chem., Cent. Drug Res. Inst., Lucknow, 226 001, India

SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1987), 26B(6), 556-61 CODEN: IJSBDB; ISSN: 0376-4699

DT Journal

LA English

OS CASREACT 108:150408

The hitherto unreported ring closure reaction of dihydropyrimidinethiones I [R = Ph, 3,4-(MeO)2C6H3, 4-MeOC6H4, 3-MeC6H4] with ClCH2CO2H in the presence of BF3·OEt2 gave dihydrothiazolo[3,2-a]pyrimidines II in 45-60% yields. Synthesis of a number of tetrasubstituted dihydropyrimidines is also reported. None of the compds. exhibit any anthelmintic activity.

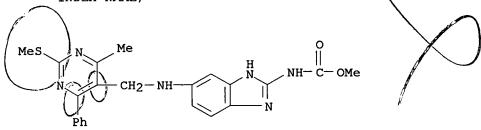
IT 113697-50-0P
RL: BAC (Biological

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and anthelmintic activity of)

RN 113697-50-0 CAPLUS

CN Carbamic acid, [5-[[[4-methyl-2-(methylthio)-6-phenyl-5-pyrimidinyl]methyl]amino]-1H-benzimidazol-2-yl]-, methyl ester (9CI) (CA INDEX NAME)



IT 113697-49-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, catalytic reduction, and cyclocondensation reaction of, with thiourea derivative)

RN 113697-49-7 CAPLUS

CN 1,4-Benzenediamine, N4-[[4-methyl-2-(methylthio)-6-phenyl-5-pyrimidinyl]methyl]-2-nitro-(9CI) (CA INDEX NAME)

- L10 ANSWER 109 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1987:138466 CAPLUS
- DN 106:138466
- TI Preparation of hydroxy- and alkoxypyrimidines as antiallergics and antiinflammatories.
- IN Lamattina, John Lawrence; Walker, Frederick J.
- PA Pfizer Inc., USA
- SO Eur. Pat. Appl., 32 pp.
 - CODEN: EPXXDW
- DT Patent
- LA English
- FAN.CNT 1

FAN.	CNT 1				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	EP 210044	 A2	19870128	EP 1986-305466	19860716
	EP 210044	A3	19871021	21 1300 000100	15000710
	EP 210044	B1	19900829		/
				LI, LU, NL, SE	/
	US 4711888	A	19871208	US 1985-758199	19850724
	AT 55995	E	19900915	AT 1986-305466	19860716
	IL 79471	_ A1	19910816	IL 1986-79471	19860721
	CA 1265519	A1	19900206	CA 1986-514336	19860722
	CN 86104539	A	19870121	CN 1986-104539	19860723
	CN 1006792	·B	19900214		
	DK 8603494	Α	19870125	DK 1986-3494	19860723
	DK 162986	В	19920106		
	DK 162986	С	19920601		
	FI 8603029	Α	19870125	FI 1986-3029	19860723
	FI 89911	В	19930831		
	FI 89911	С	19931210		
	NO 8602956	Α	19870126	NO 1986-2956	19860723
	NO 173442	В	19930906		
	NO 173442	С	19931215		
	AU 8660447	A1	19870430	AU 1986-60447	19860723
	AU 569194	B2	19880121		
	HU 41745	A2	19870528	HU 1986-3000	19860723
	HU 196764	В	19890130		
	DD 248588	A5	19870812	DD 1986-292804	19860723
	ES 2000734	. A6	19880316	ES 1986-529	19860723
	ZA 8605489	Α	19880330	ZA 1986-5489	19860723
	SU 1574171	A3	19900623	SU 1986-4027808	19860723
	JP 62026276	A2	19870204	JP 1986-174704	19860724
	JP 06047579	B4	19940622		
	PL 150617	В1	19900630	PL 1986-260784	19860724
	PL 151571	В1	19900928	PL 1986-271856	19860724
PRAI	US 1985-758199	Α	19850724		
	EP 1986-305466	Α	19860716		

Pyrimidines I [R1 = H, alkyl; R2 = H, alkyl, cyclopentyl or -hexyl, alkenyl, Ph, (un) substituted phenylalkyl; NR1R2 = (un) substituted pyrrolidino, piperidino; R3 = alkyl, Ph, (un) substituted phenylalkyl, furyl, thienyl; R4, R5 = H, alkyl, Ph, (un) substituted phenylalkyl; some restrictions apply to R1, R2, and R3] are prepared as pharmaceuticals for the title conditions (no data). Reduction of I (R1 = H, R2 = 4-ClC6H4CH2CH2CO, R3 = R4 = Me, R5 = Ac) with Dibal in THF at -23° gave 37% I [R1 = R5 = H, R2 = 4-ClC6H4(CH2)3, R3 = R4 = Me].

IT 107361-59-1P 107361-65-9P 107361-83-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as antiallergic and antiinflammatory agent)

RN 107361-59-1 CAPLUS

CN 5-Pyrimidinol, 2-[[3-(4-chlorophenyl)propyl]amino]-4-phenyl- (9CI) (CA INDEX NAME)

RN 107361-65-9 CAPLUS

CN 5-Pyrimidinol, 4-(2-fluorophenyl)-2-[(6-phenylhexyl)amino]- (9CI) (CA INDEX NAME)

RN 107361-83-1 CAPLUS

CN 5-Pyrimidinol, 4-phenyl-2-[(6-phenylhexyl)amino]- (9CI) (CA INDEX NAME)

NH- (CH₂)
$$_{6}$$
- Ph

L10 ANSWER 110 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1986:406471 CAPLUS

DN 105:6471

TI Reactions of polarized ketene S,N-acetals with guanidine: a facile general route to novel 5,6-substituted 2-amino-4-N-alkyl/aryl/N-azacycloalkylaminopyrimidines. Part XLIV

AU Vishwakarma, J. N.; Apparao, S.; Ila, H.; Junjappa, H.

CS Dep. Chem., North-Eastern Hill Univ., Shillong, 793 003, India

SO Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1985), 24B(5), 466-71 CODEN: IJSBDB; ISSN: 0376-4699

DT Journal

LA English

OS CASREACT 105:6471

AB Cyclization of polarized ketene S,N-acetals, e.g., I (R = substituted Ph; R1 = Et, Pr, PhCH2), with guanidine nitrate in Me3COH/NaOCMe3 gave the title pyrimidines, e.g., II.

RN 101476-59-9 CAPLUS

CN 2,4-Pyrimidinediamine, 6-(4-chlorophenyl)-5-nitroso-N4-(phenylmethyl)-(9CI) (CA INDEX NAME)

IT 101460-10-0P 101460-11-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 101460-10-0 CAPLUS

CN 2,4-Pyrimidinediamine, 6-phenyl-N4-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 101460-11-1 CAPLUS

CN 2,4-Pyrimidinediamine, 6-(4-chlorophenyl)-N4-(phenylmethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 111 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1986:188149 CAPLUS

DN 104:188149

TI Azo dyes for polyamide fibers and leather

IN Lamm, Gunther

PA BASF A.-G., Fed. Rep. Ger.

SO Ger. Offen., 34 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

F	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
E	PI DE 3405859	A1	19850822	DE 1984-3405859	19840218
	EP 154816	A2	19850918	EP 1985-101428	19850211/
	EP 154816	A 3	19860827		#
	EP 154816	B1	19881214		//
	R: CH, DE, FR,	GB, IT	r, LI		II .
	US 4652633	Α	19870324	US 1985-702067	19850215
	JP 60188469	A2	19850925	JP 1985-28503	19850218
E	PRAI DE 1984-3405859	Α	19840218		
_					

OS MARPAT 104:188149

AB Azo dyes of general structure I are prepared, where R = F, Br, Cl, Me, CF3, Cl-4 alkylsulfonyl, arylsulfonyl, Ac, or Bz; Rl = H, F, Cl, Br, Cl-4 alkylsulfonyl, Me, or CF3; R2 = H, Me, or Cl; and Q is the residue of a hydroxypyridone, diaminocyanopyridine, or diaminopyrimidine type coupler. I are fast, level dyes for nylon fiber and wool, and are especially suitable for

trichromatic dyeing; some also can be used as leather dyes. Thus, diazotization of 2,4,6-Cl2(HO3S)C6H2NH2 and coupling with 2,6-bis(3-hydroxypropylamino)-3-cyano-4-methylpyridine gave I (R = R1 = Cl, R2 = H, Q = Ql) (II), a lightfast, deep golden yellow dye for nylon 6 and wool. II also shows high migration and good dyeing properties in combination with red and blue dyes on nylon 6. I (R = R1 = Cl, R2 = H, Q = Q2) (Li salt; lemon yellow on leather), I (R = R1 = Cl, R2 = H, Q = Q3) (Na salt; golden yellow on nylon and wool), and numerous other yellow to orange dyes were prepared

IT 101045-17-4 101045-26-5 101045-27-6

RL: TEM (Technical or engineered material use); USES (Uses) (dye, for polyamides)

RN 101045-17-4 CAPLUS

CN Benzenesulfonic acid, 3,5-dichloro-2-[[4-[(2-hydroxyethyl)amino]-2-(3-methylphenyl)-6-[[2-(4-sulfophenyl)ethyl]amino]-5-pyrimidinyl]azo]- (9CI) (CA INDEX NAME)

RN 101045-26-5 CAPLUS

CN Benzenesulfonic acid, 5-chloro-2-[[4-[(2-hydroxyethyl)amino]-2-(3-methylphenyl)-6-[[(4-sulfophenyl)methyl]amino]-5-pyrimidinyl]azo]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)

RN 101045-27-6 CAPLUS

CN Benzenesulfonic acid, 3,5-dichloro-2-[[4-[(2-methoxy-1-methylethyl)amino]-2-phenyl-6-[[2-(4-sulfophenyl)ethyl]amino]-5-pyrimidinyl]azo]- (9CI) (CA INDEX NAME)

L10 ANSWER 112 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1986:68809 CAPLUS

DN 104:68809

TI Regiospecific synthesis of N-1 and N-2 substituted pyrimidinones employing a novel 1,3-oxazine preparation

AU Skulnick, Harvey I.; Wierenga, Wendell

CS Cancer Viral Dis. Res., Upjohn Co., Kalamazoo, MI, 49001, USA

SO Heterocycles (1985), 23(7), 1685-9 CODEN: HTCYAM; ISSN: 0385-5414

DT Journal

LA English

OS CASREACT 104:68809

AB Pyrimidinones I (R = Me, PhCH2, OH) and II (R1 = Me, HOCH2CH2CH2, Ph) were prepared from PhCOCH2CO2Et and MeSC(:NH)NH2·H2SO4 via oxazinone III.

III was treated with RNH2 to give I. Hydrolysis of III with 10% HCl gave the oxazinedione IV which was treated with R1NH2 to give II (R1 = Me, HOCH2CH2CH2). Treatment of IV with PhNH2 afforded PhNHCONHCOCH2COPh which was cyclized with polyphosphoric acid to give II.

IT 100008-31-9P

RN 100008-31-9 CAPLUS

CN 4(1H)-Pyrimidinone, 6-phenyl-2-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)



L10 ANSWER 113 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1984:591821 CAPLUS

DN 101:191821

Dihydropyrimidines and related structures. I. N2-Substituted 2-pyrimidinamines and dihydro-2-pyrimidinamines by reaction of phenylbutenones and monosubstituted guanidines

AU Wendelin, Winfried; Schermanz, Karl

CS Inst. Pharm. Chem., Univ. Graz, Graz, A-8010, Austria

SO Journal of Heterocyclic Chemistry (1984), 21(1), 65-9 CODEN: JHTCAD; ISSN: 0022-152X

DT Journal

LA English

OS CASREACT 101:191821

AB H2NC(:NH)NHR (R = Me, PhCH2) reacted with PhCH:CHCOMe and H2NC(:NH)NHCH2Ph with PhCOCH:CHMe under atmospheric O to give pyrimidine I (R = Me, PhCH2). Dihydropyrimidines II, probable intermediates in the reaction, could not be isolated. Heating H2NC(:NH)NHRCR (R = Ph, p-MeOC6H4) with PhCH:CHCOMe gave II. II (R = Ph) reacted with MeOH to give pyrimidinamine III. I (R = Ph) was heated to give I (R = Ph). The low stability of II is attributed to their strong basicity.

IT 89242-69-3P 89242-70-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 89242-69-3 CAPLUS

CN 2-Pyrimidinamine, 4-methyl-6-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 89242-70-6 CAPLUS

CN 2-Pyrimidinamine, 4-methyl-6-phenyl-N-(phenylmethyl)-, compd. with 2,4,6-trinitrophenol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 89242-69-3 CMF C18 H17 N3

CM 2

CRN 88-89-1

L10 ANSWER 114 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1984:121009 CAPLUS

DN 100:121009

TI Heterocycles. 76. Reactions of monosubstituted guanidines with 1-phenyl-1,3-butanedione

AU Wendelin, Winfried; Schermanz, Karl; Schweiger, Klaus; Fuchsgruber, Alfred

CS Inst. Pharm. Chem., Univ. Graz, Graz, A-8010, Austria

SO Monatshefte fuer Chemie (1983), 114(12), 1371-9 CODEN: MOCMB7; ISSN: 0026-9247

DT Journal

LA German

OS CASREACT 100:121009

AB H2NC(:NH)NHR (R = Me, CH2Ph, Ph) react with PhCOCH2COMe to yield exclusively pyrimidinamines I. The formation of pyrimidinimines was observed The structure of I (R = Ph) was determined by comparison with an authentic sample prepared from the pyrimidinthione II via the methylthiopyrimidine. Boiling II with PhNH2-BuOH yields the thiodipyrimidine III.

IT 89242-69-3P 89242-70-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 89242-69-3 CAPLUS

CN 2-Pyrimidinamine, 4-methyl-6-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

5 me #113

RN 89242-70-6 CAPLUS

CN 2-Pyrimidinamine, 4-methyl-6-phenyl-N-(phenylmethyl)-, compd. with 2,4,6-trinitrophenol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 89242-69-3 CMF C18 H17 N3

CM 2

CRN 88-89-1 CMF C6 H3 N3 O7

L10 ANSWER 115 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1983:594921 CAPLUS

DN 99:194921

TI Reaction of ketenethioacetals with carboxamides

AU Kohra, Shinya; Tominaga, Yoshinori; Matsuda, Yoshiro; Kobayashi, Goro

CS Fac. Pharm. Sci., Nagasaki Univ., Nagasaki, 852, Japan

SO Heterocycles (1983), 20(9), 1745-50 CODEN: HTCYAM; ISSN: 0385-5414

DT Journal

LA English

OS CASREACT 99:194921

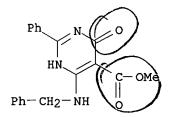
AB (MeS)2C:C(CN)CO2Me reacted with RCONH2 [I; R = Me, ClCH2, Ph, 4-R1C6H4, PhCH:CH2 (Rl = Me, OMe, Cl, NO2)] in the presence of NaH to give RCONHC(SMe):C(CN)CO2Me (II), which cyclized on refluxing in MeOH to give III (R2 = CO2Me). (MeS)2C:C(CN)2 underwent direct cyclocondensed with I to give III (R2 = CN). II (R = Ph) underwent cyclocondensed with HNR3R4 (R3 = H, R4 = Ph, PhCH2, cyclohexyl; NR3R4 = morpholino) to give IV. IV (R3 = H, R4 = Ph) cyclyzed in refluxing Ph2O to give V.

IT 87694-01-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 87694-01-7 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 1,4-dihydro-4-oxo-2-phenyl-6-[(phenylmethyl)amino]-, methyl ester (9CI) (CA INDEX NAME)





L10 ANSWER 116 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1982:423815 CAPLUS

DN 97:23815

7,8-Dihydro-2,5,8-trisubstituted-7-oxopyrido[2,3-d]pyrimidine-6-TIcarboxamides

Scotese, Anthony C.; Morris, Robert L.; Santilli, Arthur A. IN

PA American Home Products Corp., USA

SO U.S., 14 pp. Cont.-in-part of U.S. 4,215,216. CODEN: USXXAM

DTPatent

LΑ English

FAN.CNT 3

1.1	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4301281	Α	19811117	US 1980-125620	19800228
	US 4215216 JP 55141485	A A2	19800729 19801105	US 1979-31256 JP 1980-50214	19790418
	CA 1120475	A2 A1	19820323	CA 1980-350056	19800419
PRAI	US 1979-31256	A2	19790418		
	US 1980-116123	A	19800128		
os	US 1980-125620 CASREACT 97:23815	Α	19800228		.1

AB Carboxamides I [R = H, OH, C1-6 alkyl, alkylthio, Ph, 4-MeOC6H4, 4-C1C6H4, 1-pyrrolidinyl, MePhN; R1 = OH, (di) C1-6 alkylamino,, HOCH2CH2NH, C3-8 2-alkoxyethylamino, 4-methyl-1-piperazinyl, 4-morpholinyl, 1-pyrrolidinyl, NH2; R2 = (di)(C1-6 alkyl) amino; R3 = H, C1-6 alkyl, C3-6 alkoxyethyl, allyl, propargyl, Ph, 4-MeOC6H4, 4-ClC6H4, PhCH2, 4-MeOC6H4CH2, 4-ClC6H4CH2, 4-(4-morpholinyl)phenyl, piperonyl], useful as gastric antisecretory agents and in suppression of allergic manifestations in warm-blooded animals, were prepared Also prepared were esters I (R2 = C1-6 alkoxy). Aminating chloropyrimidinecarboxylate II (R4 = C1) with EtNH2 in

EtOH containing Na2CO3 overnight at room temperature, then 1 h at reflux gave

amine

derivative II (R4 = EtNH) which was cyclized with Et02CCH2COCl in Et20 in 3 h at room temperature, then treated with Na in EtOH to give pyridopyrimidinecarboxylate I (R = Ph, R1 = OH, R2 = OEt, R3 = Et) (III). At 32 mg/kg (rat) intraduodenal, III gave 45% inhibition of gastric total acid output; at 50 mg/kg i.p. or orally, III inhibited 99% allergy response in sensitized rats.

IT 76360-73-1P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclization of, with Et chloroformate, pyrimidooxazinedione derivative by)

RN 76360-73-1 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[[(4-methoxyphenyl)methyl]amino]-2-phenyl-(CA INDEX NAME) (9CI)

ΙT 76360-67-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation and cyclization of, with Et malonyl chloride, pyridopyrimidinecarboxylate derivative by)

RN 76360-67-3 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 2-phenyl-4-[(phenylmethyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{Ph} & \text{N} & \\ & \text{N} & \\ \text{Ph-CH}_2-\text{NH} & \text{O} \end{array}$$

IT 76360-72-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and saponification of)

RN 76360-72-0 CAPLUS

L10 ANSWER 117 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1982:85504 CAPLUS

DN 96:85504

TI Alkylation and acylation of 2-aminopyrimidine N-oxides

AU Sedova, V. F.; Mustafina, T. Yu.; Mamaev, V. P.

CS Novosib. Inst. Org. Khim., Novosibirsk, 630090, USSR

SO Khimiya Geterotsiklicheskikh Soedinenii (1981), (11), 1515-22 CODEN: KGSSAQ; ISSN: 0453-8234

DT Journal

LA Russian

OS CASREACT 96:85504

AB Acylation of 2-aminopyrimidines, e.g., I (R1 = R2 = H, Me; R1 = Ph, R2 = H) gave the products of O- and N-acylation; with alkylating agents only the products of O-alkylation were obtained. Reaction of 2-aminopyrimidine N-oxides with aldehydes gave only the products of amino group reaction. The structure of the obtained products depended on the reactivity of the carbonyl component.

IT 80830-66-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 80830-66-6 CAPLUS

CN 2-Pyrimidinamine, 4-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 118 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1981:139730 CAPLUS

DN 94:139730

TI Syntheses with nitriles. 60. Preparation of 4-amino-5-cyano-6-phenylpyrimidines from 2-amino-1,1-dicyano-2-phenylethene

AU Mittelbach, Martin; Junek, Hans

CS Inst. Org. Chem., Univ. Graz, Graz, A-8010, Austria

SO Journal of Heterocyclic Chemistry (1980), 17(7), 1385-7 CODEN: JHTCAD; ISSN: 0022-152X

DT Journal

LA English

OS CASREACT 94:139730

AB The reaction of 2-amino-1,1-dicyanobut-1-ene and 2-amino-1,1-dicyano-2-phenylethene, resp., with DMF dimethylacetal provided the corresponding (N,N-dimethylaminomethylene)amino derivs. 2-[(N,N-Dimethylaminomethylene)amino]-1,1-dicyano-2-phenylethene was converted into 4-amino-5-cyano-6-phenylpyrimidines, e.g. I, by treatment with primary aliphatic and aromatic amines. The structure of the reaction products was confirmed by 13C NMR spectroscopy.

IT 76990-15-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 76990-15-3 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-phenyl-6-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)



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L10 ANSWER 119 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
    1981:65719 CAPLUS
ΑN
    94:65719
DИ
    7,8-Dihydro-2,5,8-trisubstituted-7-oxo-pyrido[2,3-d]pyrimidine-6-
ΤI
    carboxylic acid derivatives
    Morris, Robert L.; Santilli, Arthur A.; Scotese, Anthony C.
IN
    American Home Products Corp., USA
PA
SO
    U.S., 14 pp.
    CODEN: USXXAM
DT
    Patent
    English
LΑ
FAN.CNT 3
                        KIND
                                          APPLICATION NO.
                                                                  DATE
    PATENT NO.
                               DATE
                        ____
                                                                  _____
                                                                  19790418
    US 4215216
                         Α
                               19800729
                                           US 1979-31256
PΙ
                                           US 1979-89065
                                                                  19791029
    US 4233446
                         Α
                               19801111
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                                                                  19791029
    US 4255568
                         Α
                               19810310
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                               19811117
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                                                                  19800403
    EP 18139
                         A2
                               19801029
    EP 18139
                         A3
                               19810107
    EP 18139
                         В1
                               19830504
        R: AT, BE, CH, DE, FR, IT, LU, NL, SE
                                           GB 1980-11250
                                                                  19800403
    GB 2048859
                         Α
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    GB 2048859
                         B2
                               19830427
                                           AT 1980-301075
                                                                  19800403
    AT 3208
                         E
                               19830515
                        Α
                                           ZA 1980-2047
                                                                  19800408
    ZA 8002047
                               19811125
                        A2
    JP 55141485
                               19801105
                                           JP 1980-50214
                                                                  19800415
    CA 1120475
                        A1
                               19820323
                                           CA 1980-350056
                                                                  19800417
                        A3
PRAI US 1979-31256
                               19790418
                               19800128
    US 1980-116123
                        Α
    US 1980-125620
                         Α
                               19800228
                         Α
                               19800403
    EP 1980-301075
    MARPAT 94:65719
OS
    Pyrido[2,3-d]pyrimidines I [R = H, OH, C1-6 alkyl, C1-6 alkylthio, Ph,
AΒ
     4-MeOC6H4, 4-ClC6H4, 1-pyrrolidinyl, MePhNH; R1 = HO, Cl-6 alkylamino,
     2-HOCH2CH2NH, C3-8 2-alkoxyethylamino, C1-6 dialkylamino, heterocyclyl; R2
     = C1-6 alkoxy, 2-HOCH2CH2NH2, 2-alkoxy- and 2-(dialkylamino)ethylamino; R3
     = H, C1-6 alkyl, C3-6 2-alkoxyethyl, allyl, propargyl, Ph, 4-tolyl,
     4-C1C6H4, PhCH2, 4-MeOC6H4CH2, 4-C1C6H4CH2, 4-morpholinophenyl, piperonyl]
    were prepared by several methods, e.g., successive aminolysis of
    pyrimidinecarboxylate II (R4 = C1), cyclocondensation with ClCOCH2COR2,
     chlorination, and further aminolysis. Thus, treating II (R = Ph, R4 = Cl)
    with EtNH2 (g) gave II (R4 = EtNH), whose cyclocondensation with
     ClCH2CO2Et gave I (R = Ph, R1 = OH, R2 = OEt, R3 = Et)(III). Treating III
     with POC13 and then with pyrrolidine gave I (R1 = 1-pyrrolidiny1). At 32
    mg/kg id. IV had 45% antigastric secretory activity and at 50 mg/kg p.o.
    had 99% antiallergy activity.
IT
     76360-73-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation and cyclocondensation of, with Et chloroformate,
        pyrimidooxazinedione derivative by)
RN
     76360-73-1 CAPLUS
     5-Pyrimidinecarboxylic acid, 4-[[(4-methoxyphenyl)methyl]amino]-2-phenyl-
CN
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(9CI) (CA INDEX NAME)

IT 76360-67-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclocondensation of, with Et malonyl chloride)

RN 76360-67-3 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 2-phenyl-4-[(phenylmethyl)amino]-, ethyl ester (9CI) (CA INDEX MAME)

IT 76360-72-0P

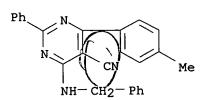
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and deesterification of)

RN 76360-72-0 CAPLUS

- L10 ANSWER 120 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1980:408129 CAPLUS
- DN 93:8129
- TI 2,6-disubstituted 4-(benzylamino)-5-cyanopyrimidines a new series of pyrimidine derivatives
- AU Robev, S.
- CS Dep. Pharmacol. Phythother., Fac. Med., Sofia, 1431, Bulg.
- Doklady Bolgarskoi Akademii Nauk (1979), 32(9), 1235-8 CODEN: DBANAD; ISSN: 0366-8681
- DT Journal
- LA English
- Pyrimidines I (R = Ph, 4-MeC6H4, 2-naphthyl, R1 = H, Cl) were obtained in 48-70% yield by cycloaddn. of 4-R1C6H4CH2N:CPhNH2 with RCH:C(CN)2, oxidation, and Dimroth rearrangement. I (R = Ph, R1 = H) was hydrolyzed by H3PO4 to 2,6-diphenyl-4(3H)-pyrimidinone.
- RN 73885-40-2 CAPLUS
- CN 5-Pyrimidinecarbonitrile, 2,4-diphenyl-6-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

- IT 73885-41-3P 73885-42-4P 73885-43-5P
 - 73885-45-7P 73885-46-8P
 - RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
- RN 73885-41-3 CAPLUS
- CN 5-Pyrimidinecarbonitrile, 4-(4-methylphenyl)-2-phenyl-6-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)



- RN 73885-42-4 CAPLUS
- CN 5-Pyrimidinecarbonitrile, 4-(2-naphthalenyl)-2-phenyl-6-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 73885-43-5 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-[[(4-chlorophenyl)methyl]amino]-2,6-diphenyl-(9CI) (CA INDEX NAME)

RN 73885-45-7 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-[[(4-chlorophenyl)methyl]amino]-6-(4-methylphenyl)-2-phenyl- (9CI) (CA INDEX NAME)

RN 73885-46-8 CAPLUS

CN 5-Pyrimidinecarbonitrile, 4-[[(4-chlorophenyl)methyl]amino]-6-(2-naphthalenyl)-2-phenyl- (9CI) (CA INDEX NAME)

L10 ANSWER 121 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1980:34952 CAPLUS

DN 92:34952

TI Correlation analysis of pyrimidine folic acid antagonists as antibacterial agents. II. Classification by mode of action using discriminant analysis

AU Smith, Carl C.; Genther, Clara S.; Coats, Eugene A.

CS Dep. Environ. Health, Univ. Cincinnati, Cincinnati, OH, 45267, USA

SO European Journal of Medicinal Chemistry (1979), 14(3), 271-6 CODEN: EJMCA5; ISSN: 0009-4374

DT Journal

LA English

The ability of folic acid [59-30-3] or folinic acid [58-05-9] to reverse the inhibitory effect of pyrimidines against Streptococcus faecium, Lactobacillus casei, and Pediococcus cerevisiae was studied. an amino group at the 2-position of the pyrimidine nucleus was related to reversible antifolate action in all 3 organisms Ph or anilino substituents at the 6-position resulted in irreversible antibacterial activity against L. casei and P cerevisiae, but was not significant against S. faecium. Discriminant anal. as an adjunct to regression anal. in characterization of structure-activity relations of pyrimidines in quant. terms is discussed.

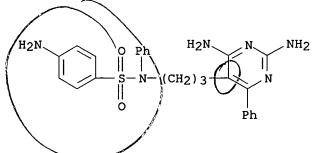
IT 71525-22-9

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(bactericidal activity of, folate reversal of, structure in relation to)

RN 71525-22-9 CAPLUS

CN Benzenesulfonamide, 4-amino-N-[3-(2,4-diamino-6-phenyl-5-pyrimidinyl)propyl]-N-phenyl- (9CI) (CA INDEX NAME)





L10 ANSWER 122 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1980:34951 CAPLUS

DN 92:34951

TI Correlation analysis of pyrimidine folic acid antagonists as antibacterial agents. I

AU Coats, Eugene A.; Genther, Clara S.; Smith, Carl C.

CS Coll. Pharm., Univ. Cincinnati, Cincinnati, OH, 45267, USA

SO European Journal of Medicinal Chemistry (1979), 14(3), 261-70 CODEN: EJMCA5; ISSN: 0009-4374

DT Journal

LA English

The activities of 175 pyrimidines as inhibitors of Streptococcus faecium, Lactobacillus casei, and Pediococcus cerevisiae are reported. In addition, the mode of action according to the ability of folic acid [59-30-3] or folinic acid [58-05-9] to reverse the inhibitory effect of the pyrimidines was determined The 2,4-diamino substituent pattern appeared to be the dominant but not the sole factor controlling mode of action. Quant. structure-activity relations using regression anal., substituent consts., and indicator variables were developed in an effort to delineate influences on potency and to quant. differences between the test systems. Although aromatic and(or) lipophilic substituents at the 5 position of 2,4-diaminopyrimidines enhanced folate reversible inhibition against all 3 systems the derived equations quant. establish differences in and limitations on the extent of this effect.

IT **71525-22-9**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(bactericidal activity of, structure in relation to)

RN 71525-22-9 CAPLUS

CN Benzenesulfonamide, 4-amino-N-[3-(2,4-diamino-6-phenyl-5-pyrimidinyl)propyl]-N-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 123 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1978:190753 CAPLUS

DN 88:190753

TI Synthesis of purines by cyclization of the Michael-type adducts from 6-aminopyrimidines and 4-phenyl-1,2,4-triazoline-3,5-dione

AU Yoneda, Fumio; Kawamura, Mitsuko; Matsumoto, Shiqeru; Higuchi, Masatsugu

CS Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, Japan

SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1977), (20), 2285-8 CODEN: JCPRB4; ISSN: 0300-922X

DT Journal

LA English

OS CASREACT 88:190753

The Michael-type adducts I (R = H, Me, R1 = Me, R2 = H, CH2Ph; R = Me, R1 = H, R2 = Me, Pr, Bu) and II [R = Me, R1 = Pr, Bu, CH2Ph, (CH2)2Ph; R = Ph, R1 = CH2Ph] were prepared by treatment of the corresponding uracils with 4-phenyl-1,2,4-triazoline-3,5-dione. Oxidative cyclization of I (R = H, Me, R1 = Me, R2 = CH2Ph) with PhNO2 gave the corresponding xanthines III (R3 = Ph), which were also obtained, together with III (R = R1 = Me, R3 = 3,4-Cl2C6H3, 4-ClC6H4, 4-MeOC6H4, 4-Me2NC6H4; R = H, R1 = Me, R3 = 4-ClC6H4, 3,4-Cl2C6H3), by condensation of I (R = H, Me, R1 = Me, R2 = H) with R3CHO. Direct cyclization of the Michael-type adducts II [R = Me, R1 = CH2Ph, (CH2)2Ph; R = Ph, R1 = CH2Ph] with PhNO2 gave the corresponding purines IV.

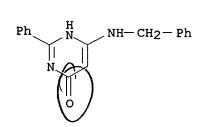
IT 66487-67-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and Michael addition reaction of, with phenyltriazolinedione)

RN 66487-67-0 CAPLUS

CN 4(1H)-Pyrimidinone, 2-phenyl-6-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)





IT 66487-61-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and oxidative cyclization of)

RN 66487-61-4 CAPLUS

CN 1,2,4-Triazolidine-3,5-dione, 1-[1,4-dihydro-4-oxo-2-phenyl-6-[(phenylmethyl)amino]-5-pyrimidinyl]-4-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 124 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1978:105255 CAPLUS

DN 88:105255

TI Displacement reactions of 2-alkylsulfonyl-4-chloropyrimidine derivatives with nucleophiles

AU Sawayama, Tadahiro; Yamamoto, Ryuichi; Kinugasa, Hiroaki; Nishimura, Haruki

CS Res. Lab., Dainippon Pharm. Co., Ltd., Suita, Japan

SO Heterocycles (1977), 8, 299-305 CODEN: HTCYAM; ISSN: 0385-5414

DT Journal

LA English

OS CASREACT 88:105255

AB Aminolysis of chloropyrimidines I [R = Ph, H, R1 = Et, R2 = Cl; R = R1 = Me, R2 = Cl) gave I (R2 = NH2, NHCH2Ph, NHMe, NHPh, morpholino, piperidino, 4-methylpiperazino, 4-(2-hydroxyethyl)piperazino] and II (R = same; R3 = SO2R1, Cl; R4 = H, CH2Ph, Me, Ph). 4-Chloro-2-ethoxy-6-phenylpyrimidine was obtained as a by-product of the ammonolysis of I (R = Ph, R1 = Et, R2 = Cl) in EtOH.

IT 65766-20-3P 65766-22-5P 65766-26-9P
RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 65766-20-3 CAPLUS

CN 2-Pyrimidinamine, 4-chloro-6-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 65766-22-5 CAPLUS

CN 4-Pyrimidinamine, 2-(ethylsulfonyl)-6-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 65766-26-9 CAPLUS

CN 2-Pyrimidinamine, 4-(ethylsulfonyl)-6-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 125 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1977:171488 CAPLUS

86:171488 DN

Substituted-2-(pyrimidinylthio)acetamidoximes and acetonitriles ΤI

Santilli, Arthur A.; Scotese, Anthony C. IN

American Home Products Corp., USA PA

SO U.S., 5 pp. CODEN: USXXAM

DΤ Patent

LΑ English

FAN

FAN.CNT 1				
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3950339	Α	19760413	US 1975-570546	19750422 /
DDAT HC 1074_514676	7.2	107/1015		/

PRAI US 1974-514676 A2 19741015

Six acetamidoximes I (R = p-ClC6H4CH2, 1,3-benzodioxol-5-ylmethyl, p-MeOC6H4; R1 = Me, Pr, Ph), with antiarrhythmic activity in dogs, were prepared by reaction of acetonitriles II (R1 as before; R2 = RNH; R as before) with NH2OH.HCl in DMF in the presence of Na2CO3 at elevated temperature II (R2 = RNH) were prepared by reaction of RNH2 with II (R2 = Cl), which were obtained by condensing 6-substituted 2-thiouracil Na salts with C1CH2CONH2 and treating the resultant (pyrimidinylthio)acetamides with POC13.

IT 56605-25-5P

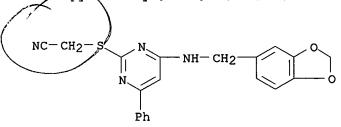
> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with hydroxylamine hydrochloride)

RN 56605-25-5 CAPLUS

Acetonitrile, [[4-[(1,3-benzodioxol-5-ylmethyl)amino]-6-phenyl-2-CN

pyrimidinyl]thio]- (9CI) (CA INDEX NAME)

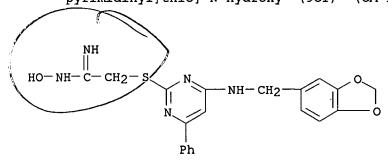


ΙT 56605-34-6P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, for use as antiarrhythmic agent)

RN 56605-34-6 CAPLUS

Ethanimidamide, 2-[[4-[(1,3-benzodioxol-5-ylmethyl)amino]-6-phenyl-2-CN pyrimidinyl]thio]-N-hydroxy- (9CI) (CA INDEX NAME)



L10 ANSWER 126 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1976:478077 CAPLUS

DN 85:78077

TI Methylation of 4-amino-5-phenylpyrimidine and proof of the structure of its derivatives

AU Tsatsaronis, G.; Soulis, T.

CS Lab. Org. Chem. Technol. Food Chem., Univ. Thessaloniki, Salonika, Greece

SO Prakt. Panelleniou Chem. Synedriou, 4th (1972), Meeting Date 1970, Volume 1, 64-8 Publisher: Chem. Chron., Athens, Greece.

CODEN: 32PRAD

DT Conference

LA Greek

AB Alkylation of 4-amino-5-phenylpyrimidine with R2SO4 (R = Me, Et) afforded products alkylated in the 1-position, which gave the corresponding imines I when treated with NaOH. II was obtained by treatment of I (R = Me) with hot or cold alkali. Reaction of MeNHCHO with PhCH(CN)CH:NH gave 4-methylamino-5-phenylpyrimidine. Reaction of 4-chloro-5-phenyl(or p-nitrophenyl)pyrimidine with R1NH2 (R1 = Et, Pr, Bu, cyclohexyl, PhCH2) gave 21-63% III (same R1; R2 = H, NO2).

IT 60122-84-1P 60122-87-4P

RN 60122-84-1 CAPLUS

CN 4-Pyrimidinamine, 5-phenyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 60122-87-4 CAPLUS

CN 4-Pyrimidinamine, 5-(4-nitrophenyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

L10 ANSWER 127 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1976:38578 CAPLUS

DN 84:38578

TI Correlation analysis of Baker's studies on enzyme inhibition. 2. Chymotrypsin, trypsin, thymidine phosphorylase, uridine phosphorylase, thymidilate synthetase, cytosine nucleoside deaminase, dihydrofolate reductase, malate, glutamate, lactate, and glyceraldehyde-phosphate dehydrogenase

AU Yoshimoto, Masafumi; Hansch, Corwin

CS Dep. Chem., Pomona Coll., Claremont, CA, USA

SO Journal of Medicinal Chemistry (1976), 19(1), 71-98 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

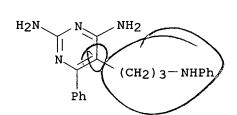
The inhibitory activity of .apprx.1000 inhibitors of the title enzymes, $\alpha\text{-chymotrypsin}$ [9004-07-3], trypsin [9002-07-7], thymidine phosphorylase [9030-23-3], uridine phosphorylase [9030-22-2], thymidylate synthetase [9031-61-2], cytosine nucleoside deaminase [9025-06-3], dihydrofolate reductase [9002-03-3], malate dehydrogenase [9001-64-3], glutamate dehydrogenase [9001-46-1], glyceraldehyde-phosphate dehydrogenase [9001-50-7], and lactate dehydrogenase [9001-60-9], were formulated in 13 equations correlating chemical structure with inhibiting potency. Two types of regions in enzymes were defined by means of π and molar refractive consts. The correlation equations showed that substituent effects are additive to a 1st approximation Examples are given of use of the equations in comparing structural features of different systems.

IT 2211-01-0

RL: BIOL (Biological study)
(dihydrofolate reductase inhibition by, correlation anal. in relation to)

RN 2211-01-0 CAPLUS

CN 2,4-Pyrimidinediamine, 6-phenyl-5-[3-(phenylamino)propyl]- (9CI) (CA INDEX NAME)





L10 ANSWER 128 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1975:578969 CAPLUS

DN 83:178969

TI Synthesis of 5,6,7,8-tetrahydro-5-oxopyrido[2,3-d]pyrimidine-6-carbonitriles and -6-carboxylic acid esters

AU Santilli, Arthur A.; Wanser, Stephen V.; Kim, Dong H.; Scotese, Anthony C.

CS Res. Dev. Div., Wyeth Lab. Inc., Radnor, PA, USA

SO Journal of Heterocyclic Chemistry (1975), 12(2), 311-16 CODEN: JHTCAD; ISSN: 0022-152X

DT Journal

LA English

OS CASREACT 83:178969

AB 5-Carbethoxy-4-chloro-2-phenylpyrimidine was treated with RNHCH2CH2CN (R = Me, PhCH2CH2, morpholinoethyl, etc.) to give I, which underwent ring closure to give II (R1 = H). II (R = Me, R1 = H) was methylated to give II (R = R1 = Me). II (R = Me, R1 = H) and p-MeC6H4SO2Cl gave III. II (R = Me, R1 = H) and SOCl2 gave IV. Several similar pyridopyrimidines were also prepared

IT 35855-41-5P 35855-45-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclization of, pyridopyrimidinecarbonitriles from)

RN 35855-41-5 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[(2-cyanoethyl)(2-phenylethyl)amino]-2-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 35855-45-9 CAPLUS

$$C1$$
 CH_2-CH_2-CN
 CH_2-N-R

L10 ANSWER 129 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1975:557714 CAPLUS

DN 83:157714

TI Synthesis and antiarrhythmic activity of substituted (2-pyrimidinylthio) acetamidoximes

AU Scotese, Anthony C.; Santilli, Arthur A.; Nelson, George L.

CS Res. Dev. Div., Wyeth Lab., Inc., Radnor, PA, USA

SO Journal of Medicinal Chemistry (1975), 18(8), 852-4 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

OS CASREACT 83:157714

AB Of 17 title acetamidoximes and acetonitrile intermediates, prepared by S-alkylation of the 6-substituted thiouracil with 2-chloroacetamide [79-07-2], dehydration to the nitrile and replacement of the 4-OH group by Cl by treatment with POCl3, amination and treatment with hydroxylamine, 5 compds. had significant activity in the antiarrhythmic screen in dogs. 2-[4-Methyl-6-(p-chlorobenzylamino)-2-pyrimidinylthio]acetamidoxime-2HCl (I-2HCl) [56605-29-9] was the most potent antiarrhythmic agent. Structure-activity relations are discussed.

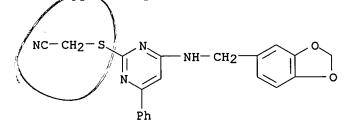
IT 56605-25-5P 56605-32-4P 56605-34-6P

56641-09-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation and antiarrhythmic activity of)

RN 56605-25-5 CAPLUS

CN Acetonitrile, [[4-[(1,3-benzodioxol-5-ylmethyl)amino]-6-phenyl-2-pyrimidinyl]thio]- (9CI) (CA INDEX NAME)



RN 56605-32-4 CAPLUS

CN Ethanimidamide, 2-[[4-[[(4-chlorophenyl)methyl]amino]-6-phenyl-2-pyrimidinyl]thio]-N-hydroxy- (9CI) (CA INDEX NAME)

RN 56605-34-6 CAPLUS

CN Ethanimidamide, 2-[[4-[(1,3-benzodioxol-5-ylmethyl)amino]-6-phenyl-2-pyrimidinyl]thio]-N-hydroxy- (9CI) (CA INDEX NAME)

$$\begin{array}{c} NH \\ \parallel \\ HO-NH-C-CH_2-S \\ \hline N \\ N \\ \hline NH-CH_2 \\ \hline O \\ O \\ \end{array}$$

RN 56641-09-9 CAPLUS

CN Acetonitrile, [[4-[[(4-chlorophenyl)methyl]amino]-6-phenyl-2-pyrimidinyl]thio]- (9CI) (CA INDEX NAME)

L10 ANSWER 130 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1975:43455 CAPLUS

DN 82:43455

TI 5,6,7,8-Tetrahydro-5-oxo-pyrido(2,3-d)pyrimidine-6-carbonitriles and related compounds

IN Santilli, Arthur A.; Kim, Dong H.

PA American Home Products Corp.

SO U.S., 6 pp. Division of U.S. 3,726,869 (CA 78: 159653x). CODEN: USXXAM

DT Patent

LA English

FAN.CNT 4

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 3843645	Α	19741022	US 1972-310311	19721129
US 3726869	Α	19730410	US 1971-136997	19710423
PRAI US 1971-136997	A 3	19710423		
US 1968-752485	A3	19680814		<i>y</i>

AB The pyridopyrimidines I (R = Me, CH2CH2Ph, morpholinoethyl, CH2CH2OMe, CH2C6H4Cl-p) were prepared by treating the chloropyrimidine II with RNHCH2CH2CN and cyclizing with NaOEt. I were central nervous system depressants in mice at 12.7-40 mg/kg i.p.

IT 35855-41-5P 35855-45-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclization of)

RN 35855-41-5 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[(2-cyanoethyl)(2-phenylethyl)amino]-2-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} & \text{N} \\ & \text{N} & \text{C-OEt} \\ \text{NC-CH}_2\text{-CH}_2\text{-N} & \text{O} \\ & \text{Ph-CH}_2\text{-CH}_2 \end{array}$$

RN 35855-45-9 CAPLUS

$$\begin{array}{c|c} \operatorname{CH}_2-\operatorname{CH}_2-\operatorname{CN} \\ & | \\ \operatorname{CH}_2-\operatorname{N}-\operatorname{R} \end{array}$$

L10 ANSWER 131 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1973:432081 CAPLUS

DN 79:32081

TI 4-[(2-Cyanoethyl)amino]-2-phenyl-5-pyrimidinecarboxylic acid esters

IN Santilli, Arthur A.; Kim, Dong H.

PA American Home Products Corp.

SO U.S., 5 pp. Division of U.S. 3,641,027 (CA 76;127008h). CODEN: USXXAM

DT Patent

LA English

FAN. CNT 4

LTIV.	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	us 3732226	Α	19730508	us 1971-136670	19710423
	US 3641027	A	19720208	US 1968-752485	19680814/
DDAT	TIS 1968-752485	A3	19680814		A

The pyrido[2,3-d]pyrimidinecarbonitriles I (R = Me, PhCH2CH2, morpholinoethyl, MeOCH2CH2, p-ClC6H4CH2) were prepared by cyclization of the pyrimidinecarboxylates II. Thus, 5-carbethoxy-4-chloro-2-phenylpyrimidine was treated with MeNHCH2CH2CN to give II (R = Me) which was heated in EtOH containing EtONa to give I (R = Me). I were depressants at 12.7-40 mg/kg.

IT 35855-41-5P 35855-45-9P

RN 35855-41-5 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[(2-cyanoethyl)(2-phenylethyl)amino]-2-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} & \text{N} \\ & \text{N} & \text{C-OEt} \\ \text{NC-CH}_2\text{-CH}_2\text{-N} & \text{O} \\ & \text{Ph-CH}_2\text{-CH}_2 \end{array}$$

RN 35855-45-9 CAPLUS

$$\begin{array}{c|c} \text{CH}_2\text{--}\text{CH}_2\text{--}\text{CN} \\ & \downarrow \\ \text{CH}_2\text{--}\text{N}\text{---}\text{R} \end{array}$$

L10 ANSWER 132 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1972:127008 CAPLUS

DN 76:127008

TI 5,6,7,8-Tetrahydro-5-oxopyrido[2,3-d]pyrimidine-6-carbonitriles and related compounds

IN Santilli, Arthur A.; Kim, Dong H.

PA American Home Products Corp.

SO U.S., 5 pp. CODEN: USXXAM

DT Patent

LA English

FAN. CNT 4

FAN.CNI 4						
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
PI US 3641027	A	19720208	US 1968-752485	19680814		
US 3726869	A	19730410	US 1971-136997	19710423		
US 3732226	Α	19730508	US 1971-136670	19710423/		
PRAI US 1968-752485	A 3	19680814				

5-Carbethoxy-4-chloro-2-phenylpyrimidine was treated with MeNH(CH2)2CN and Na2CO3 to give I (R = Me) (II). Five similar I (R = Ph(CH2)2, 2-morpholinoethyl, MeO(CH2)2, Et2N(CH2)2, p-ClC6H4CH2) were prepared II was treated with NaOEt to give the pyrido[2,3-d]pyrimidine (III, R = Me). Four similar III (R = Ph(CH2)2, 2-morpholinoethyl, MeO(CH2)2, p-ClC6H4CH2) were prepared I and III were depressants.

IT 35855-41-5P 35855-45-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 35855-41-5 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[(2-cyanoethyl)(2-phenylethyl)amino]-2-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 35855-45-9 CAPLUS

$$\begin{array}{c|c} \operatorname{CH}_2-\operatorname{CH}_2-\operatorname{CN} \\ & | \\ & | \\ \operatorname{CH}_2-\operatorname{N---} R \end{array}$$

L10 ANSWER 133 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1972:82480 CAPLUS

DN 76:82480

TI Role of folate coenzymes in the initiation of protein synthesis

AU Dickerman, Herbert W.

CS Sch. Med., Johns Hopkins Univ., Baltimore, MD, USA

SO Annals of the New York Academy of Sciences (1971), 186, 70-81 CODEN: ANYAA9; ISSN: 0077-8923

DT Journal

LA English

AB Methionyl tRNAfMet was characterized by its activity as a substrate in the formylation reaction; its participation, as the N-formyl derivative, in the formation of the initiation complex; and its exclusion from participation in the transfer complex. Methionyl tRNAfMet transformylase, approx. 90% pure, had a slightly acidic isoelec. point, a mol. weight of approx. 25,000 daltons, and was not a cationic protein like the histones. 44 references.

IT 35960-68-0

RL: BIOL (Biological study)

(methionyl ribonucleic acid formylation by transformylase inhibition by)

RN 35960-68-0 CAPLUS

CN L-Glutamic acid, N-[4-[[3-(2-amino-1,4-dihydro-4-oxo-6-phenyl-5-pyrimidinyl)propyl]amino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L10 ANSWER 134 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1972:34229 CAPLUS

DN 76:34229

TI Syntheses of N-heterocyclic compounds. II. Pyrimido[4,5-e]-, pyridazino[3,4-e]-, and pyrido[4,3-e]-1,2,3,5-tetrahydro[1,4]oxazepin-5-one

AU Yuruqi, Shojiro; Hieda, Masaru; Fushimi, Tomiyoshi; Tomimoto, Mitsumi

CS Res. Dev. Div., Takeda Chem. Ind., Ltd., Osaka, Japan

SO Chemical & Pharmaceutical Bulletin (1971), 19(11), 2354-64 CODEN: CPBTAL; ISSN: 0009-2363

DT Journal

LA English

Pyrimido[4,5-e][1,4]oxazepines were synthesized by the reaction of 2-substituted-4-chloro-5-ethoxycarbonylpyrimidines with N-substituted ethanolamines. The reaction was applied to the syntheses of the pyridazo[3,4-e]-[1,4]oxazepines and pyrido[4,3-e][1,4]oxazepines. In the course of this study a N-O rearrangement at the 4-position of 2-phenyl-4-(N-phenyl-2-hydroxyethylamino)-5-ethoxycarbonylpyrimidine was observed

IT 34750-69-1P 34753-26-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 34750-69-1 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 4-[(2-hydroxyethyl)(phenylmethyl)amino]-2-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} & \text{N} \\ & \text{N} & \text{C-OEt} \\ & \text{HO-CH}_2\text{-CH}_2\text{-N} & \text{O} \\ & \text{Ph-CH}_2 & \end{array}$$

RN 34753-26-9 CAPLUS

CN 5-Pyrimidinecarboxamide, 2-phenyl-N-(phenylmethyl)-4-[(phenylmethyl)amino](9CI) (CA INDEX NAME)

L10 ANSWER 135 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1970:79077 CAPLUS

DN 72:79077

TI Coccidiostatic N-[(2-substituted-4-aminopyrimidinyl)methyl]-3-ethoxy-4-alkoxycarbonylanilinium bromide hydrobromides

PA Chimetron S.a r.l.

SO Fr., 4 pp.

CODEN: FRXXAK

DT Patent

LA French

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1566160		19690509	FR	19660527

PI FR 1566160 19690509 FR 19660527

AB The title compds. (I), useful as coccidiostats, are prepared by treating 4-amino-5-(halomethyl)pyrimidines with 4-amino-2-ethoxybenzoic acids. Thus, 0.1 mole 2-propyl-4-amino-5-(bromomethyl)-pyrimidine was treated with 0.1 mole of Me 4-amino-2-ethoxybenzoate in 250 ml iso-PrOH and 50 ml 2M HBr added to give I (R = Pr, R1 = Me, X = Br).HBr.

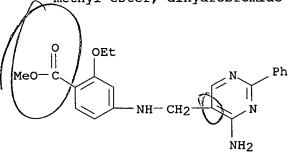
2-Ethyl-4-amino-5-(bromomethyl)pyrimidine (0.1 mole) in 300 ml MeCN was treated with 27.6 g Me 4-amino-2-ethoxybenzoate-HBr and the mixture refluxed 1 hr to give I (R = R1 = Et, X = Br).HBr.

IT 26667-80-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 26667-80-1 CAPLUS

CN Benzoic acid, 4-[[(4-amino-2-phenyl-5-pyrimidinyl)methyl]amino]-2-ethoxy-, methyl ester, dihydrobromide (8CI) (CA INDEX NAME)



•2 HBr

L10 ANSWER 136 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1968:400301 CAPLUS

DN 69:301

TI Irreversible enzyme inhibitors. CXIX. Active-site-directed irreversible inhibitors of dihydrofolic reductase with tissue specificity derived from 2,4,6-triaminopyrimidine with a terminal sulfonyl fluoride at the 5 position

AU Baker, Bernard Randall; Meyer, Rich B., Jr.

CS Univ. of California Santa Barbara, Santa Barbara, CA, USA

SO Journal of Medicinal Chemistry (1968), 11(3), 489-94 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

AΒ Four derivs. of 5-phenoxypropyl-2,4,6-triaminopyrimidine with the following substituents on the para position were synthesized as candidate active-site-directed irreversible inhibitors of dihydrofolic reductase: m-fluorosulfonylbenzamido (I), ρ -fluorosulfonylbenzamido (II), m-fluorosulfonylphenylureido (III), and ρ -fluorosulfonyl-phenylureido (IV). At a concentration near 1 μ M, I could rapidly inactivate the dihydrofolic reductase from Walker 256 rat tumor and L1210/FR8 mouse leukemia, but showed little irreversible inhibition of the enzyme from rat liver, mouse liver, or L1210/0. This specificity for rat tumor enzyme over rat liver enzyme was considerably decreased when the carboxamido group of I was lengthened to ureido (III), the tumor enzyme being inactivated about four-fold faster than the rat liver enzyme; however, specificity of inactivation of the L1210/FR8 enzyme by III with no irreversible inhibition of the mouse liver enzyme was maintained. Movement of the sulfonyl fluoride from the meta position of I and III to give II and IV resulted in considerably slower irreversible inhibitors; since the enzyme could apparently catalyze hydrolysis of the sulfonyl fluoride of II and IV to the irreversibly ineffective sulfonic acid more rapidly, the amount of irreversible inhibition was also decreased. references.

IT 20768-17-6P 20768-18-7P

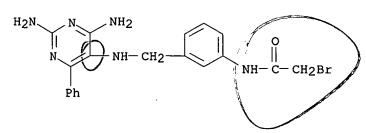
RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 20768-17-6 CAPLUS

CN m-Acetotoluidide, 2-bromo- α -[(2,4-diamino-6-phenyl-5-pyrimidinyl)amino]-, monopicrate (8CI) (CA INDEX NAME)

CM 1

CRN 47539-37-7 CMF C19 H19 Br N6 O



CM 2

CRN 88-89-1

CMF C6 H3 N3 O7

RN 20768-18-7 CAPLUS CN p-Acetotoluidide, 2-bromo- α -[(2,4-diamino-6-phenyl-5-pyrimidinyl)amino]-, monopicrate (8CI) (CA INDEX NAME)

CM 1

CRN 47539-38-8 CMF C19 H19 Br N6 O

CM 2

CRN 88-89-1 CMF C6 H3 N3 O7

L10 ANSWER 137 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1968:400299 CAPLUS

DN 69:299

TI Irreversible enzyme inhibitors. CXVI. Active-site-directed irreversible inhibitors of dihydrofolic reductase derived from 6-substituted 2,4-diamino-5-phenylpyrimidines. 3

AU Baker, Bernard Randall; Huang, Ping Cheong; Meyer, Rich B., Jr.

CS Univ. of California, Santa Barbara, CA, USA

SO Journal of Medicinal Chemistry (1968), 11(3), 475-82 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

Ten candidate irreversible inhibitors derived from 5-(p-chlorophenyl)-AΒ 2,4-diaminopyrimidine bearing a leaving group on a chain at the 6 position were evaluated on dihydrofolic reductase from Walker 256 rat tumor and L1210/FR8 mouse leukemia; three had a chloromethyl, 4 had a sulfonyl fluoride, and 3 had a bromoacetamido leaving group. Strong evidence was obtained that the diaminopyrimidine could complex as one of 2 rotomers depending upon the hydrophobicity of the group at the 6 position; 6-phenoxymethyl- and 6-phenethylpyrimidines were bound in a conformation giving a hydrophobic interaction of the 6 group with the enzyme, but the more polar 6-anilinomethyl-pyrimidines were bound in a flipped-over conformation. Three of the sulfonyl fluorides, 6-[m-(mfluorosulfonylphenylureido) - phenoxymethyl]-2,4-diamino-5-(ρchlorophenyl) pyrimidine (I), the 5-(3,4-dichlorophenyl) analog of I, and the phenethyl analog of I, were good active-site-directed irreversible inhibitors of dihydrofolic reductase. 22 references.

IT 20535-55-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 20535-55-1 CAPLUS

CN Pyrimidine, 2,4-diamino-6-[[p-[2-(chloromethyl)-1,3-dioxolan-2-yl]anilino]methyl]-5-(3,4-dichlorophenyl)- (8CI) (CA INDEX NAME)



IT 20535-88-0P

RN

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of and tetrahydrofolate dehydrogenase inhibition by) 20535-88-0 CAPLUS

CN Acetophenone, 2-chloro-4'-[[[2,6-diamino-5-(3,4-dichlorophenyl)-4-pyrimidinyl]methyl]amino]-, monohydrochloride (8CI) (CA INDEX NAME)

● HCl

L10 ANSWER 138 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1968:27157 CAPLUS

DN 68:27157

TI Irreversible enzyme inhibitors. CVIII. 6-(p-Chloroacetylanilinomethyl)-5-(p-chlorophenyl)-2,4-diaminopyrimidine, an active-site-directed irreversible inhibitor of dihydrofolic reductase

AU Baker, Bernard Randall; Huang, Ping Cheong; Pogolotti, Alfonso L., Jr.

CS Univ. of California, Santa Barbara, CA, USA

SO Journal of Medicinal Chemistry (1967), 10(6), 1134-8 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

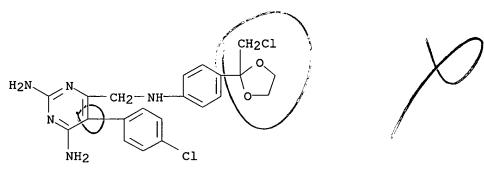
AB The title compound (I) was synthesized by reductive condensation of 5-(p-chlorophenyl)-2,4-diaminopyrimidine-6-carboxaldehyde with <math>2-(p-aminophenyl)-2-chloromethyl-1,3-dioxolane followed by hydrolysis of the ketal blocking group. Three higher homologs were also synthesized from the appropriate 2-(p-aminophenylalkyl)-2-chloromethyl-1,3-dioxolane. I rapidly inactivated the dihydrofolic reductase from Walker 256 rat tumor, rat liver, and mouse leukemia L1210/FR8; the enzyme from pigeon liver was inactivated perceptibly slower. That reversible complex formation between the enzyme and the inhibitor was a necessary prerequisite for inactivation was shown by the failure of $p-amino-\alpha-chloroacetophenone$ to inactivate dihydrofolic reductase under conditions that led to rapid inactivation with I. 22 references.

IT 18861-36-4P 18861-37-5P 18861-38-6P 18861-39-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 18861-36-4 CAPLUS

CN Pyrimidine, 2,4-diamino-6-[[p-[2-(chloromethyl)-1,3-dioxolan-2-yl]anilino]methyl]-5-(p-chlorophenyl)- (8CI) (CA INDEX NAME)



RN 18861-37-5 CAPLUS

CN Pyrimidine, 2,4-diamino-6-[[p-[2-[2-(chloromethyl)-1,3-dioxolan-2-yl]vinyl]anilino]methyl]-5-(p-chlorophenyl)- (8CI) (CA INDEX NAME)

RN 18861-38-6 CAPLUS

CN Pyrimidine, 2,4-diamino-6-[[p-[2-[2-(chloromethyl)-1,3-dioxolan-2-yl]ethyl]anilino]methyl]-5-(p-chlorophenyl)- (8CI) (CA INDEX NAME)

RN 18861-39-7 CAPLUS

CN Pyrimidine, 2,4-diamino-6-[[p-[4-[2-(chloromethyl)-1,3-dioxolan-2-yl]butyl]anilino]methyl]-5-(p-chlorophenyl)- (8CI) (CA INDEX NAME)

$$H_2N$$
 N
 CH_2-NH
 $CH_$

IT 15422-30-7P 15422-31-8P 15422-32-9P

15422-33-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of and tetrahydrofolate dehydrogenase inhibition by)

RN 15422-30-7 CAPLUS

CN Ethanone, 2-chloro-1-[4-[[[2,6-diamino-5-(4-chlorophenyl)-4-pyrimidinyl]methyl]amino]phenyl]- (9CI) (CA INDEX NAME)

$$R$$
 CH_2-NH
 R
 $C-CH_2C1$
 NH_2
 O

RN 15422-31-8 CAPLUS

CN 2-Butanone, 1-chloro-4-[[[[2,6-diamino-5-(4-chlorophenyl)-4-pyrimidinyl]methyl]amino]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \mathbf{H_2N} & \mathbf{N} & \mathbf{CH_2-NH} & \mathbf{O} \\ \mathbf{N} & \mathbf{R} & \mathbf{CH_2-CH_2-C-CH_2C1} \\ \mathbf{NH_2} & \mathbf{CH_2-CH_2-C-CH_2C1} \end{array}$$

RN 15422-32-9 CAPLUS

CN 2-Hexanone, 1-chloro-6-[4-[[[2,6-diamino-5-(4-chlorophenyl)-4-pyrimidinyl]methyl]amino]phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & & & & & & & & & & & & & \\ & & & & & & & & & & & & & \\ & & & & & & & & & & & \\ & & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & & \\ & & & & & & & & \\ & & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & \\ & & \\ & & \\ & \\ & \\ & \\ & & \\ &$$

RN 15422-33-0 CAPLUS

CN 3-Buten-2-one, 1-chloro-4-[[[[2,6-diamino-5-(4-chlorophenyl)-4-

pyrimidinyl]methyl]amino]phenyl] - (9CI) (CA INDEX NAME)

$$R$$
 CH_2
 CH_2
 CH_2
 CH_3
 CH_4
 CH_5
 CH_6
 CH_7
 $CH_$

L10 ANSWER 139 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1967:418079 CAPLUS

DN 67:18079

TI Irreversible enzyme inhibitors. LXXXV. On the mode of pyrimidine binding of 5-alkyl and 5-arylpyrimidines to dihydrofolic reductase

AU Baker, Bernard Randall; Lourens, Gerhardus J.; Jordaan, Johannes H.

CS Univ. of California, Santa Barbara, CA, USA

SO Journal of Heterocyclic Chemistry (1967), 4(1), 39-48 CODEN: JHTCAD; ISSN: 0022-152X

DT Journal

LA English

cf. preceding abstract A series of 5-isoamyl- and 5-(p-AΒ chlorophenyl)pyrimidines substituted with amino, alkylamino, mercapto, benzyloxy, hydroxy, or hydrogen at the 2- and 4-positions and with amino or methyl at the 6-position have been synthesized for evaluation of the mode of pyrimidine binding to dihydrofolic reductase. The studies were performed in order to determine where a bulky group could be placed on the pyrimidine ring that would still allow good binding; such studies are essential to find a suitable position for placement of a covalent forming group for design of active-site-directed irreversible inhibitors. Two classes of candidate compds. have emerged for further study as irreversible inhibitors, namely, 2-amino-4-mercapto-6-(pbromoacetamidophenylalkyl)pyrimidines (I) and 2,4-diamino-6-(pbromoacetamidophenylalkyl)aminopyrimidines having a group such as phenyl, phenylbutyl or isoamyl at the 5-position that can give strong hydrophobic bonding to the enzyme. 27 references.

IT 17005-50-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of and tetrahydrofolate dehydrogenase inhibition by)

RN 17005-50-4 CAPLUS

CN Pyrimidine, 2-amino-5-(p-chlorophenyl)-4-methyl-6-[(3-phenylpropyl)amino]-(8CI) (CA INDEX NAME)



L10 ANSWER 140 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1967:418076 CAPLUS

DN 67:18076

TI Irreversible enzyme inhibitors. LXXXII. Candidate active-site-directed irreversible inhibitors of dihydrofolic reductase. 7. Derivatives of 2,4-diaminopyrimidine I

AU Baker, Bernard Randall; Jackson, Graham D. F.; Meyers, Rich B., Jr.

CS Univ. of California, Santa Barbara, CA, USA

SO Journal of Pharmaceutical Sciences (1967), 56(5), 566-70 CODEN: JPMSAE; ISSN: 0022-3549

DT Journal

LA English

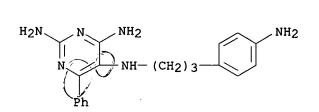
AB cf. preceding abstract Fusion of α-benzoyl-α- (phenylazo)acetonitrile with guanidine carbonate gave 2,4-diamino-6-phenyl-5-phenylazopyrimidine (I) in 52% yield; catalytic reduction of I to 6-phenyl-2,4,5-triaminopyrimidine (II) proceeded smoothly. Condensation of the triaminopyrimidine (II) with p-nitrocinnamaldehyde to an anil, followed by a 2-stage reduction, afforded 5-(p-aminophenylpropylamino)-2,4-diamino-6-phenylpyrimidine; selective bromoacetylation on the p-amino group gave the candidate irreversible inhibitor, 5-(p-bromoacetamidophenylpropylamino)-2,4 - diamino - 6 - phenylpyrimidine (III). When III was incubated with dihydrofolic reductase in the presence or absence of TPNH, no inactivation occurred; the possible conformational differences in binding to dihydrofolic reductase between III and other successful activesite-directed irreversible inhibitors are discussed.

IT 13491-73-1P 17005-17-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of and tetrahydrofolate dehydrogenase inhibition by)

RN 13491-73-1 CAPLUS

CN 2,4,5-Pyrimidinetriamine, N5-[3-(4-aminophenyl)propyl]-6-phenyl- (9CI) (CA INDEX NAME)





RN 17005-17-3 CAPLUS

CN Acetanilide, 2-bromo-4'-[3-[(2,4-diamino-6-phenyl-5-pyrimidinyl)amino]propyl]-, monopicrate (8CI) (CA INDEX NAME)

CM 1

CRN 13491-74-2

CMF C21 H23 Br N6 O

CM 2

CRN 88-89-1 CMF C6 H3 N3 O7

$$O_2N$$
 O_2
 O_1
 O_2
 O_1
 O_2

L10 ANSWER 141 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1967:62159 CAPLUS

DN 66:62159

TI Structure-activity analysis of tetrahydrofolate analogs using substituent constants and regression analysis

AU Miller, Elinor; Hansch, Corwin

CS Pomona Coll., Claremont, CA, USA

SO Journal of Pharmaceutical Sciences (1967), 56(1), 92-7 CODEN: JPMSAE; ISSN: 0022-3549

DT Journal

LA English

AB The binding to dihydrofolate reductase of a series of substituted pyrimidines and triazines is dependent on the electron-contributing and lipophilic character of the substituents. The configuration of binding is variable, and is determined by the necessity of placing the most lipophilic substituent in a hydrophobic region of the enzyme. When two or more lipophilic substituents are present, competition between them for the hydrophobic site is dominated by the more lipophilic group, while the less lipophilic group contributes to hydrophobic bonding to a slight extent. Suggestions are made for the design of a new tetrahydrofolate analog with possible application as a nonclassical antimetabolite. 24 references.

IT 2211-01-0

RL: PROC (Process)

(structure-activity anal. of)

RN 2211-01-0 CAPLUS

CN 2,4-Pyrimidinediamine, 6-phenyl-5-[3-(phenylamino)propyl]- (9CI) (CA INDEX NAME)



L10 ANSWER 142 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1967:62157 CAPLUS

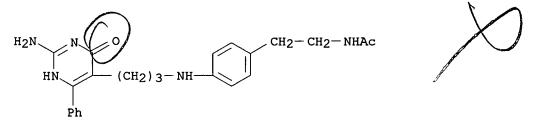
DN 66:62157

- TI Irreversible enzyme inhibitors LXXI. Candidate active-site-directed irreversible inhibitors of dihydrofolic reductase. 5. Derivatives of 6-phenylpyrimidine
- AU Baker, Bernard Randall; Shapiro, Howard S.
- CS Univ. of California, Santa Barbara, CA, USA
- SO Journal of Pharmaceutical Sciences (1967), 56(1), 33-8 CODEN: JPMSAE; ISSN: 0022-3549
- DT Journal
- LA English
- AB cf. preceding abstract A series of 2-amino-5-(anilinopropyl)-6-phenyl-4pyrimidinols bearing p-chloroacetyl, p-(4-chloro-3-butanon-1-yl) (I), p-(4-chloro-1-buten-3-on-1-yl) (II), and p-bromoacetamidoethyl (III) groups on the anilino moiety were synthesized as candidate active-site-directed irreversible inhibitors of dihydrofolic reductase. Only I inactivated dihydrofolic reductase when they were incubated together at 37°; the half-life was about 60 min. when sufficient I was utilized to convert 45% of the enzyme to a reversible complex. this inactivation by I proceeded through a reversible enzyme-inhibitor complex and not by a random bimol. mechanism was indicated by the lack of inactivation of dihydrofolic reductase by chloroacetone at 2.5 times the concentration of I. The failure of II and III to inactivate the enzyme at a concentration sufficient to convert 50-60% of the enzyme to the respective reversible complexes indicated that the alkylating function of II and III could not bridge to a nucleophilic site on the enzyme within the enzyme-inhibitor complex. 34 references.
- IT 15473-88-8P 15946-59-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 15473-88-8 CAPLUS

CN Acetamide, N-[p-[[3-(2-amino-4-hydroxy-6-phenyl-5-pyrimidinyl)propyl]amino]phenethyl]- (8CI) (CA INDEX NAME)



RN 15946-59-5 CAPLUS

CN 4-Pyrimidinol, 2-amino-5-[3-[p-(2-aminoethyl)anilino]propyl]-6-phenyl-, monohydrochloride (8CI) (CA INDEX NAME)

$$H_2N$$
 N
 O
 $CH_2-CH_2-NH_2$
 HN
 Ph

HC1

IT 15473-84-4 15473-85-5 15473-86-6

15473-87-7

RL: BIOL (Biological study)

(tetrahydrofolate dehydrogenase inhibition by, active-site-directed irreversible inhibition in relation to)

RN 15473-84-4 CAPLUS

CN Acetamide, N-[2-[4-[[3-(2-amino-1,4-dihydro-4-oxo-6-phenyl-5-pyrimidinyl)propyl]amino]phenyl]ethyl]-2-bromo-(9CI) (CA INDEX NAME)

$$H_2N$$
 H_2N
 H_2N
 H_2N
 H_3
 H_4
 H_4
 H_5
 H_5
 H_6
 H_7
 H_8
 H_8

RN 15473-85-5 CAPLUS

CN 4(1H)-Pyrimidinone, 2-amino-5-[3-[[4-(chloroacetyl)phenyl]amino]propyl]-6-phenyl- (9CI) (CA INDEX NAME)

$$H_2N$$
 N
 O
 $C-CH_2C1$
 Ph

RN 15473-86-6 CAPLUS

CN 4(1H)-Pyrimidinone, 2-amino-5-[3-[[4-(4-chloro-3-oxo-1-butenyl)phenyl]amino]propyl]-6-phenyl- (9CI) (CA INDEX NAME)

$$H_2N$$
 H_2N
 $CH = CH - C - CH_2C1$
 $CH_2O = CH - C - CH_2C1$

RN 15473-87-7 CAPLUS
CN 4(3H)-Pyrimidinone, 2-amino-5-[3-[p-(4-chloro-3-oxobutyl)anilino]propyl]-6-phenyl- (8CI) (CA INDEX NAME)

L10 ANSWER 143 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1967:37878 CAPLUS

DN 66:37878

TI Analogs of tetrahydrofolic acid. XXXIX. Selective bromoacylation of polyfunctional molecules for synthesis of active-site-directed irreversible enzyme inhibitors

AU Baker, Bernard Randall; Santi, Daniel V.; Coward, James K.; Shapiro, Howard S.; Jordaan, Johannes H.

CS Univ. of California, Santa Barbara, CA, USA

SO Journal of Heterocyclic Chemistry (1966), 3(4), 425-34 CODEN: JHTCAD; ISSN: 0022-152X

DT Journal

LA English

AB cf. CA 65, 2558b, 18581e. A number of methods for selective bromoacylation of side-chain amino groups on 2-amino-4-pyrimidinols (I) or 2,4,6-triaminopyrimidines were developed for these extremely sensitive products. The choice of method depends upon whether (a) the aminopyrimidine is a stronger base than the amine to be bromoacylated, (b) as weak a base as the amine to be bromoacylated but the amine is more reactive, (c) the amine group to be bromoacylated is a strong aliphatic amine. In case (a) the aminopyrimidine can be protonated to protect it from acylation with an anhydride; in case (b), the reaction with an anhydride is controlled by temperature, stoichiometry, and time of reaction; in case (c), the reaction is selectively controlled by use of the less reactive p-nitrophenyl esters. Other difficulties were solved such as (a) proper characterization of the products when combustion analyses were unsatisfactory due to polymerization; in these cases a combination of thin-layer

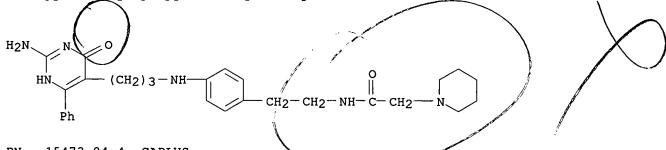
chromatography, color reactions, and derivatization were employed; and (b) insolubility leading to overreaction on the aminopyrimidine which was solved with partial aqueous systems. 38 references.

IT 13480-67-6P 15473-84-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 13480-67-6 CAPLUS

CN 1-Piperidineacetamide, N-[p-[[3-(2-amino-4-hydroxy-6-phenyl-5-pyrimidinyl)propyl]amino]phenethyl]- (8CI) (CA INDEX NAME)



RN 15473-84-4 CAPLUS

CN Acetamide, N-[2-[4-[[3-(2-amino-1,4-dihydro-4-0xo-6-phenyl-5-pyrimidinyl)propyl]amino]phenyl]ethyl]-2-bromo-(9CI) (CA INDEX NAME)

L10 ANSWER 144 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1966:106358 CAPLUS

DN 64:106358

OREF 64:20106b-c

TI Analogs of tetrahydrofolic acid. XXXIV. Hydrophobic bonding to dihydrofolic reductase. 6. Mode of phenyl binding of some 6-arylpyrimidines

AU Baker, B. R.; Shapiro, Howard S.

CS State Univ. of New York, Buffalo

SO Journal of Pharmaceutical Sciences (1966), 55(3), 308-17 CODEN: JPMSAE; ISSN: 0022-3549

DT Journal

LA English

AB cf. preceding abstrs. New data are presented which strongly support the concept that the increment in better binding observed by substituting a phenyl group on the 6-position of 4-pyrimidinol is due to hydrophobic bonding of the phenyl group. Furthermore, 11 6-phenylpyrimidines with various substituents at the 2, 4, and 5-positions were compared with 18 5-aryl-and 5-arylalkylpyrimidines as inhibitors of dihydrofolic reductase. The results cannot be explained by a single conformation of the pyrimidine being complexed to the enzyme; therefore, a number of rotational conformers for the pyrimidine ring are proposed where the strong hydrophobic bonding by the phenyl or phenylalkyl substituent is the determining factor for the particular preferred conformation of a given inhibitor. Such a hypothesis has previously been invoked to explain the inhibitor and substrate binding to chymotrypsin by Niemann, et al. (cf. Jones, et al., CA 63, 10254f).

IT 4455-56-5, Pyrimidine, 2-amino-5-(3-anilinopropyl)-4-phenyl-

(preparation of and tetrahydrofolic dehydrogenase inhibition by)

RN 4455-56-5 CAPLUS

CN 5-Pyrimidinepropanamine, 2-amino-N,4-diphenyl- (9CI) (CA INDEX NAME)

$$H_2N$$
 N
 $(CH_2)_3-NHPh$



1T 853-66-7, 4-Pyrimidinol, 2-amino-5-(3-anilinopropyl)-6-phenyl2211-01-0, Pyrimidine, 2,4-diamino-5-(3-anilinopropyl)-6-phenyl2360-67-0, 4-Pyrimidinethiol, 2-amino-5-(3-anilinopropyl)-6-phenyl-

4455-56-5, Pyrimidine, 2-amino-5-(3-anilinopropyl)-4-phenyl-(tetrahydrofolic dehydrogenase inhibition by)

RN 853-66-7 CAPLUS

CN 4(1H)-Pyrimidinone, 2-amino-6-phenyl-5-[3-(phenylamino)propyl]- (9CI) (CF INDEX NAME)

$$H_2N$$
 N
 O
 $CH_2)_3-NHPh$

RN 2211-01-0 CAPLUS

CN 2,4-Pyrimidinediamine, 6-phenyl-5-[3-(phenylamino)propyl]- (9CI) (CA INDEX NAME)

$$H_2N$$
 N
 NH_2
 $NH_$

RN 2360-67-0 CAPLUS

CN 4(1H)-Pyrimidinethione, 2-amino-6-phenyl-5-[3-(phenylamino)propyl]- (9CI) (CA INDEX NAME)

$$H_2N$$
 H_N
 S
 $(CH_2)_3-NHPh$

RN 4455-56-5 CAPLUS

CN 5-Pyrimidinepropanamine, 2-amino-N, 4-diphenyl- (9CI) (CA INDEX NAME)

L10 ANSWER 145 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1965:404573 CAPLUS

DN 63:4573

OREF 63:861e-f

TI Analogs of tetrahydrofolic acid. XVIII. On the mode of binding of some 6-aryl- and 6-aralkylpyrimidines to folic reductase

AU Baker, B. R.; Shapiro, Howard S.; Werkheiser, William C.

CS State Univ. of New York, Buffalo

SO Journal of Medicinal Chemistry (1965), 8(3), 283-7 CODEN: JMCMAR; ISSN: 0022-2623

DT Journal

LA English

AB cf. CA 62, 8048a, 14667a. A series of 2-amino-5-anilinopropyl-4-pyrimidinols bearing a p-nitrophenyl, p-tolyl, or 2-furyl group at the 6-position were synthesized. In addition, a series of 2,4-diaminopyrimidines with a phenylbutyl or anilinopropyl group at the 5-position and bearing either a 6-phenyl or 6-benzyl group were prepared Enzymic evaluation of the effects of these and related compds. on folic reductase showed that the increase in binding of 2-amino-5-(3-anilinopropyl)-6-methyl-4-pyrimidinol previously observed by single replacement of (a) the anilino group by benzyl, (b) the 6-methyl by 6-phenyl or 6-benzyl, (c) the 4-hydroxyl by 4-amino, or (d) the 4-hydroxyl by 4-mercapto were not necessarily additive if 2 or more of these changes were made in the same mol.; some cases of additivity in binding were observed with 2 structural changes.

IT 853-66-7, 4-Pyrimidinol, 2-amino-5-(3-anilinopropyl)-6-phenyl-, complex with folic reductase 2211-01-0, Pyrimidine, 2,4-diamino-5-(3-anilinopropyl)-6-phenyl-, complex with folic reductase 2257-74-1, p-Toluenesulfonanilide, N-[3-(2-amino-4-chloro-6-phenyl-5-pyrimidinyl)propyl]-, complex with folic reductase 2257-80-9, p-Toluenesulfonanilide, N-[3-(2-amino-4-hydroxy-6-p-tolyl-5-pyrimidinyl)propyl]-, complex with folic reductase 2360-67-0, 4-Pyrimidinethiol, 2-amino-5-(3-anilinopropyl)-6-phenyl-, complex with folic reductase

(preparation of)

RN 853-66-7 CAPLUS

CN 4(1H)-Pyrimidinone, 2-amino-6-phenyl-5-[3-(phenylamino)propyl]- (9CI) (CA INDEX NAME)

$$H_2N$$
 H_2N
 $(CH_2)_3-NHPh$



RN 2211-01-0 CAPLUS

CN 2,4-Pyrimidinediamine, 6-phenyl-5-[3-(phenylamino)propyl]- (9CI) (CA INDEX NAME)

$$^{\text{NH}_2\text{N}}$$
 $^{\text{NH}_2}$ $^{\text{NH}_2}$ $^{\text{CH}_2)}$ 3 $^{\text{NHPh}}$

RN 2257-74-1 CAPLUS

CN p-Toluenesulfonanilide, N-[3-(2-amino-4-chloro-6-phenyl-5-pyrimidinyl)propyl]- (8CI) (CA INDEX NAME)

RN 2257-80-9 CAPLUS

CN p-Toluenesulfonanilide, N-[3-(2-amino-4-hydroxy-6-p-tolyl-5-pyrimidinyl)propyl]- (8CI) (CA INDEX NAME)

$$\begin{array}{c|c} H_2N & H & Ph & O \\ \hline & N & R & Ph & O \\ \hline & (CH_2) & 3-N-S & O \\ \hline & O & O \\ \end{array}$$

RN 2360-67-0 CAPLUS

CN 4(1H)-Pyrimidinethione, 2-amino-6-phenyl-5-[3-(phenylamino)propyl]- (9CI) (CA INDEX NAME)

$$H_2N$$
 H_N
 S
 $(CH_2)_3-NHPh$

- L10 ANSWER 146 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
- AN 1965:43892 CAPLUS
- DN 62:43892
- OREF 62:7750g-h,7751a-h,7752a-e
- TI Analogs of tetrahydrofolic acid. XIV. Facile synthetic route to the 2-amino-5-(3-anilinopropyl)-6-methyl-4-pyrimidinol-type of folic reductase and thymidylate synthetase inhibitor
- AU Baker, B. R.; Santi, Daniel V.; Shapiro, Howard S.
- CS State Univ. of New York, Buffalo
- SO Journal of Pharmaceutical Sciences (1964), 53(11), 1317-25 CODEN: JPMSAE; ISSN: 0022-3549
- DT Journal
- LA English

with

AB cf. CA 61, 4346d. Tosylation of p-O2NC6H4NH2 with 21 g. tosyl chloride in 50 ml. pyridine gave 27.7 g. N-(p-nitrophenyl)-p-toluenesulfonamide (I), m. 193°. Similarly p-H2NC6H4.CO2Et gave N-(p-carbethoxyphenyl)-p-toluenesulfonamide (II), m. 206-7°. A solution of 2.47 g. p-toluenesulfonanilide in 10 ml. Me2SO was treated with 1.38 g. K2CO3 and 8.07 g. 1,3-dibromopropane, the mixture stirred at room temperature 3 days, added

to 75 ml. H2O, and extracted with C6H6, the benzene solution washed with NaOH, and the solvents distilled to give 2.72 g. N-(3-bromopropyl)-ptoluenesulfonanilide (III), m. 64-5°. Similarly I gave N-(3-bromopropyl)-N-(p-nitrophenyl)-p-toluenesulfonamide (IV), m. 119-20° and II gave N-(3-bromopropyl)-N-(p-carbethoxyphenyl)-ptoluenesulfonamide (V), m. 77-9°. Reaction of III with AcCH2CO2Et in EtOH proceeded poorly. Hence a mixture of 73 ml. tert-BuOH, 3.9 g. AcCH2CO2Et, and 1.43 g. NaH was warmed till the NaH dissolved completely. To this was then added 7.37 g. III and the mixture refluxed 20 hrs. to give 8.32 g. Et 2-acetyl-5-anilino-N-(p-tolylsulfonyl)valerate (VI) as a glass, 84% pure based on uv analysis. Similarly, IV gave Et 2-acetyl-5-(pnitroanilino)-N-(p-tolylsulfonyl)valerate (VII), m. 107-8°. Since VI seemed to be labile to EtOH, its use as a solvent in the next stage was avoided and tert-BuOH substituted. A mixture of 8.32 g. VI, 2 g. guanidine carbonate, and 50 ml. tert-BuOH was refluxed 48 hrs. and filtered, the precipitate dissolved in 50 ml. H2O, and the solution acidified to neutrality

HOAc and filtered to give 5.54 g. 2-amino-6-methyl-5-[N-(p-tolylsulfonylanilino)propyl]-4-pyrimidinol (VIII), m. 226-8°. Similarly, VII gave 2-amino-6-methyl-5-[N-(p-tolylsulfonyl-p-nitroanilino)-propyl]-4-pyrimidinol (IX), m. 125-55° (decomposition), and V gave 2-amino-5-[N-(p-tolylsulfonyl-p-carbethoxyanilino)propyl]-4-pyrimidinol (X) as a glass, which showed several spots in thin layer chromatography and could not be purified further. The tosyl group of VIII could not be

removed by hydrolysis with 96% H2SO4 at room temperature or with boiling concentrated

HCl; the material was recovered. Hence a solution of 1.03 g. VIII in 50 ml. liquid NH3 was treated with 340 mg. Na in small pieces when the blue color failed to fade. The mixture was then treated with 1 g. NH4Cl, NH3 removed, the residue dissolved in 25 ml. H2O, the solution acidified with HCl to pH 1 and filtered, and the filtrate treated with NaOH to pH 8 to give 0.34 g. 2-amino-6-methyl-5-(3-anilinopropyl)-4-pyrimidinol (XI), m. 219°. Alternatively, a mixture of 2.19 g. VIII, 1 g. PhOH, and 11.5 g. 30% HBr in HOAc was stirred 16 hrs. and diluted with Et2O, HBr salt filtered off and dissolved in 20 ml. 3N HCl, and the solution made slightly alkaline with NH3 to give 0.965 g. XI, m. 219-20°, identical with the above sample. Similarly IX gave 2-amino-6-methyl-5-(p-nitroanilinopropyl)-4-pyrimidinol (XII), m. 260-1°, and X gave 2-amino-6-methyl-5-(p-

carbethoxyanilinopropyl)-4-pyrimidinol (XIII), m. 194-6°. Hydrolysis of 150 mg. XIII with 5% NaOH on a steam bath 30 min. gave 104 mg. 2-amino-6-methyl-5-(p-carboxyanilinopropyl)-4-pyrimidinol, identical with a sample prepared by an earlier method (Baker et al., J. Med. Chemical, 1964, 7, 24). VIII was used to synthesize pyrimidines with a blocked anilino group, e.g., synthesis of 2,4-diamino-5-(3-anilinopropyl)-6methylpyrimidine (results to be published). Syntheses of some other blocked anilinopyrimidines were investigated. A solution of 0.294 q. Na and 1.94 q. BzCH2CO2Et in 25 ml. tert-BuOH was refluxed with III 20 hrs. and worked up as above to give 3.27 g. BzCH(CO2Et)(CH2)3N(O2SC6H4Me-p)Ph (XIV) as an oil. A solution of 3.26 g. crude XIV in 15 ml. tert-BuOH was refluxed with 0.61 g. guanidine carbonate 51 hrs. to give 0.804 g. 2-amino-6-phenyl-[N-(p-tolylsulfonyl)anilinopropyl]-4-pyrimidinol (XV), m. 222-4°. A solution of 500 mg. XV and 200 mg. PhOH in 2.3 g. 30% HBr in HOAc was kept 20 hrs. and worked up to give 300 mg. 2-amino-5-(3-anilinopropyl)-6-phenyl-4-pyrimidinol (XVI), m. 235-41° (decomposition). XVI was also obtained from known XVII(CA 59, 13979e). A solution of 2 g. XVII and 6 g. PhNH2 in 40 ml. HCONMe2 (DMF) was stirred 30 min., 300 ml. MeOH added, and the mixture treated with 4 g. NaBH4 portionwise. After stirring 18 hrs. the reaction was worked up to give 1.52 g. XVI identical with the above. Reduction of 0.5 g. XVII in 10 ml. DMF and 50 ml. MeOH with NaBH4 gave 0.349 g. 2-amino-4-hydroxy-6-phenyl-5pyrimidylpropanol, m. 265-8°. Reduction of XV with Na in liquid NH3 removed the tosyl group but the product appeared to be the 5,6-dihydro derivative of XVI since it no longer had an absorption peak at 280 mm characteristic of the 6-phenylpyrimidines. Apparently the 6-Ph substituent activated the 5,6-double bond for reduction Similar marked differences due to 6-Ph group were noticed in other compds. of this type. A homolog of XVI was also synthesized. Reaction of PhCH2COCl with Et ethoxymagnesiomalonate gave Et phenylacetylmalonate which on refluxing with H2O gave Et γ -phenylacetoacetate (XVIII), b0.05 80-107°, n22D 1.054-1.059. Refluxing 4 g. XVIII with 1.75 g. quanidine carbonate in 40 ml. MeOH gave 1.64 g. 2-amino-6-benzyl-4-pyrimidinol, m. 278-80°. Condensation of XVIII with acrolein under base-catalyzed conditions did not give the expected product, PhCH2COCH(CO2Et)CH2CH2CHO (XIX). A further aldol condensation occurred to give XX since the product showed absence of aldehyde CH absorption at 2600 cm.-1 Milder conditions gave unchanged XVIII or mixts. of XIX and XX and hence this approach was abandoned. In a second route PhCH2COCl was condensed with the Na derivative of XXI (R = Me, R1 = H) (XXII) to give XXI (R = PhCH2, R1 = Ac) XXIII). Cleavage of XXIII with NaOMe did not give the expected product XXI (R =PhCH2, R1 = H) by cleavage of the Ac group but mainly XXII by cleavage of PhCH2CO group. XXII was characterized by conversion to the 6-methylpyrimidine (XXIV). Hence the method used above for the synthesis of the title compound was used. Alkylation of 20.3 g. XVIII with 12.5 g. III followed by condensation of the product with guanidine 67 hrs. gave 7.4g. 2-amino-6-benzyl-5-(N-tosylanilinopropyl)-4-pyrimidinol (XXV), m. 133-5°. Reduction of 450 mg. XXV as described above gave 133 mg. 2-amino-5-(anilinopropyl)-6-benzyl-4-pyrimidinol (XXVI), m. 181°. Before the successful attempt to insert a 1,3-dihalopropane between an oxo ester and an aniline as outlined above, 4 other routes were investigated. The diamion of α benzoylacetanilide was prepared by heating 2 g. with 0.728 g. NaH in DMF and then treated with 1,3-dibromopropane 48 hrs. to give 0.586 g. 3-benzoyl-1-phenyl-2-piperidone (XXVII), m. 160-2°, existing probably as a stable chelate. That it was fully enolized was confirmed by its ir and N.M.R., spectra. XXVII did not react with quanidine carbonate under normal conditions and when conditions were forced, C-benzoyl cleavage took place. With guanidine hydrochloride in

polyphosphoric acid there was decomposition XXVII did not form an enol ether with Et orthoformate or Et orthoacetate. No enamine or O-mesitylate could be prepared Possibility of O-methylation with CH2N2 was not investigated. Alkylation of AcCH2CO2Et with 1-bromo-3-chloropropane in EtOH-MeONa gave only 5% yield of AcCH(CO2Et)(CH2)3Cl (XXVIII), the rest being converted to XXIX and this method was not further investigated. Reaction of the anion of PhNHAc with 1,3-dibromopropane did not give a clear cut product and the separation of desired N-(3-bromopropyl)acetanilide was not of preparative value. Reaction of PhNHMe with excess 1,3-dibromopropane gave distillable but unstable Br(CH2)3NMePh (XXX) which on redistn. or standing gave crystals of putative XXXI bromide. Reaction of XXX with Et sodioacetoacetate to prepare AcCH(CO2Et)(CH2)3NMePh failed. The ir spectra of all the compds. were described. The biol. properties were described and discussed.

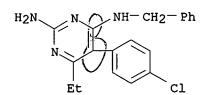
RN 853-66-7 CAPLUS

CN 4(1H)-Pyrimidinone, 2-amino-6-phenyl-5-[3-(phenylamino)propyl]- (9CI) (CA INDEX NAME)

RN 863-89-8 CAPLUS

CN p-Toluenesulfonanilide, N-[3-(2-amino-4-hydroxy-6-phenyl-5-pyrimidinyl)propyl]- (7CI, 8CI) (CA INDEX NAMÉ)

L10 ANSWER 147 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN 1956:28390 CAPLUS AN 50:28390 DN OREF 50:5779c-e Pyridine compds. Societe des usines chimiques de Rhone-Poulenc DTLA Unavailable FAN.CNT 1 PATENT NO. APPLICATION NO. DATE KIND DATE -----____ PΙ GB 731956 19550615 GB DE 1082267 DE AΒ Compds. having antimalarial properties are obtained from 2-amino-4-chloro-5-(4-chlorophenyl)-6-ethylpyrimidine (I) or its 2-AcNH analog and an amine, RNH2, or its salt, where R is a saturated or unsatd. aliphatic radical with 1-6 C atoms, cycloalkyl, or arylalkyl. I is prepared from guanidine and p-ClC6H4CH(COEt)CO2Et in 15-40% oleum, followed by treatment with POCl3. E.g., 5 g. I, 10 ml. MeNH2, and 10 ml. EtOH heated in an autoclave 7.5 hrs. at $160-5^{\circ}$, taken up in 100 ml. H2O, filtered, and the product washed with H2O and dried yielded 4.1 g. 2-amino-4-methylamino-5-(4-chlorophenyl)-6-ethylpyrimidine (II), m. 212-13°; II.HCl.H2O, m. 160° and 245-50°. II is formed also from the acyl derivative of I. The following 4-RNH analogs of II were prepared by this procedure (R and m.p. given); Et, $182-3^{\circ}$ (HCl salt-H2O, 150° and 232°); Pr, 140 and 157°; iso-Pr, 210° (HCl salt-H2O, 150 and 210°); Bu, 133° (HCl salt, 200-5°); n-pentyl, 114-15°; n-hexyl, 109-10 and
118°; "2'-butyl," 166°; "3'-butyl," 164°; isopentyl,
143°; cyclohexyl, 202° (HCl salt, 240°); allyl, 150-1°; benzyl, 140°. These compds. are also prepared from I and an amine HCl salt heated at 200° without a solvent. IT 856972-58-2, Pyrimidine, 2-amino-4-benzylamino-5-(p-chlorophenyl)-6-ethyl-(preparation of) RN 856972-58-2 CAPLUS CN Pyrimidine, 2-amino-4-benzylamino-5-(p-chlorophenyl)-6-ethyl- (5CI) (CA INDEX NAME)





L10 ANSWER 148 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN

AN 1955:60839 CAPLUS

DN 49:60839

OREF 49:11726h-i,11727a-b

TI 2-Amino-4-substituted amino-6-arylpyrimidines

IN Hitchings, Geo. H.; Russell, Peter B.

PA Burroughs Wellcome and Co. (U.S.A.) Inc.

DT Patent

LA Unavailable

FAN.CNT 1

а

PATENT NO. KIND DATE APPLICATION NO. DATE

-----PI US 2691655 19541012 US 1952-289907 19520524

AB 2-Amino-4-substituted amino-6-arylpyrimidines, useful as growth inhibit

AB 2-Amino-4-substituted amino-6-arylpyrimidines, useful as growth inhibitors for rapidly growing virus are prepared from the corresponding 4-hydroxypyrimidine by conversion to the-4-chloropyrimidine and subsequent reaction with the appropriate amine. Thus, 47 g. BzCHPrCO2Et, refluxed 6 hrs. with 12 g. guanidine carbonate in 200 ml. EtOH, gives 2-amino-4-hydroxy-5-propyl-6-phenylpyrimidine (I), m. 311-13°, obtained by dilution of the reaction mixture with 500 ml. H2O and recrystn. of the precipitate from EtOH; the 5-benzyl analog (II), m. 340°, was prepared similarly from BzCH(CH2Ph)CO2Et. Refluxing 10 g. I with 50 ml. POCl3 until solution was achieved, removing the excess POCl3, and suspending the residue in iced aqueous NH4OH gave 2-amino-4-chloro-5-propyl-6-phenylpyrimidine (III). Similarly, II yields the 5-benzyl analog (IV) of III; heating 5 g. III with 100 ml. of a saturated solution of MeNH2 in EtOH in

bomb for 16 hrs. at 150° gives 4.2 g. 4-MeNH analog of III, m. 198°, and IV gives the 4-MeNH analog of IV, m. 177°.

Refluxing 5 g. III with 25 ml. of PhNH2 5 hrs., cooling, and recrystg. the precipitate from EtOH, gives needles of the 4-PhNH analog of III, m. 171°; 4-PhNH analog of IV, m. 211°. The following compds. are obtained by analogous procedures: 2-amino-4-methylamino-6-(2-naphthyl)pyrimidine, m. 238-9°; 2-amino-4-methylamino-6-phenylpyrimidine, m. 195-6°, and its 4-PhNH, m. 305-6° (decomposition), 4-(p-ClC6H4NH), m. 304-5°, and 4-(p-MeOC6H4NH) analogs, m. 259-63°.

IT 856972-54-8, Pyrimidine, 2-amino-4-benzylamino-5-ethyl-6-(pnitrophenyl)-

(preparation of)

RN 856972-54-8 CAPLUS

CN Pyrimidine, 2-amino-4-benzylamino-5-ethyl-6-(p-nitrophenyl)- (5CI) (CA INDEX NAME)

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L10 ANSWER 149 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     1955:16281 CAPLUS
DN
     49:16281
OREF 49:3270d-h
     2-Mercapto-4-(secondary-amino)pyrimidines
ΤI
     Hitchings, Geo. H.; Russell, Peter B.
IN
PA
     Burroughs Wellcome & Co. (U.S.A.) Inc.
DT
LΑ
     Unavailable
FAN.CNT 1
     PATENT NO.
                         KIND
                                 DATE
                                             APPLICATION NO.
                                                                     DATE
                                             -----
                         ____
ΡI
     US 2671087
                                 19540302
                                             US 1951-261394
                                                                     19511212
AB
     2,4-Dimercaptopyrimidine (I) (1 mole) treated with 3 moles of primary
     amine at approx. 100° gives 80-90% corresponding
     N:C(SH).N:C(NHR).CR1:CR2 (II), where R consists of alkyl, monocyclic aryl,
     or aralkyl radicals, R1 consists of alkyl groups and H, and R2 consists of
     alkyl, monocyclic aryl and aralkyl radicals and H. II are useful
     pharmaceutical products. 5-Methyldithiouracil 1.3 g. and 10 cc. of a 33% aqueous MeNH2 solution are heated in a bomb at 100^{\circ} for 3.5 hrs., the
     contents of the tube evaporated to dryness, and the residue crystallized
several
     times from hot aqueous solution giving 60% 2-mercapto-5-methyl-4-
     methylaminopyrimidine. Similarly prepared are the following
     2-mercapto-4-aminopyrimidine derivs.: 5-amyl-N4-methyl, m. 198°;
     5-amyl-6-methyl-N4-methyl; 5-methyl-6-amyl-N4-methyl; 5-methyl-6-propyl-N4-
     methyl; 5-ethyl-6-phenyl-N4-methyl; 5-methyl-N4-tetradecyl;
     5-hexyl-N4-tetradecyl; N4,5-ditetradecyl-6-methyl; 5-methyl-6-propyl-N4-
     amyl;5-methyl-N4-benzyl; 5-ethyl-6-phenyl-N4-benzyl; 5-propyl-N4-β-
     hydroxyethyl; 5-methyl-6-phenyl-N4-β-hydroxyethyl;
     5-propyl-6-methyl-N4-phenyl; 5-methyl-6-phenyl-N4-phenyl; N4-methyl, m
     236-7°; N4-tetradecyl, m. 148-9°; N4-amyl, m. 218°;
     N4-benzyl, m. 248-9°; N4-β-methylhexyl; 6-ethyl-N4-propyl;
     6-phenyl-N4-hexyl; N4-β-diethylaminoethyl, m. 114-15°;
     N4-β-hydroxyethyl, m. 226-8°; 6-methyl-N4-phenyl, m.
     230°; 6-amyl-N4-phenyl, m. 227-8°; 6-phenyl-N4-phenyl,
     6-phenyl-N4-tetradecyl; N4-phenyl, m. 285°' N4-p-chlorophenyl, m.
     299°; 6-methyl-N4-amyl, m. 221; 6-phenyl-N4-amyl, m. 227-8°;
     and 6-phenyl-N4-p-methoxyphenyl, m. 264-5° (from
     6-phenyldithiouracil and p-methoxyaniline).
ΙT
     857412-78-3, 2-Pyrimidinethiol, 4-benzylamino-5-ethyl-6-phenyl-
        (preparation of)
RN
     857412-78-3 CAPLUS
CN
     2-Pyrimidinethiol, 4-benzylamino-5-ethyl-6-phenyl- (5CI) (CA INDEX NAME)
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L10 ANSWER 150 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
AN
    1953:28894 CAPLUS
DN
     47:28894
OREF 47:4921d-i,4922a-b
TI 4-Amino-5-arylpyrimidines
    Hitchings, Geo. H.; Russell, Peter B.; Falco, Elvira A.
IN
     Burroughs Wellcome & Co. (U.S.A.) Inc.
PA
DT
     Patent
LΑ
    Unavailable
FAN.CNT 1
                                                                    DATE
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                             _____
                         ----
                                 _____
                                19520708
                                            US
PΙ
    US 2602794
     4-Amino-5-arylpyrimidines (I) are prepared by condensing an
AΒ
     \alpha-aryl-\beta-alkoxyacrylonitrile with a suitable urea derivative, such
     as a guanidine or amidine. I are useful antimalarials and bactericides.
     2,4-Diamino-5-phenylpyrimidine is prepared in 60% yield from guanidine (II)
     and PhCH(CHO)CN in refluxing CH2N2 (III) or HC(OEt)3. The following are
     similarly prepared: 6-Methyl-2,4-diamino-5-(p-chlorophenyl)-pyrimidines, m.
     264-5° (from aqueous alc.) [60% from p-ClC6H4CHAcCN, II, and III, or
     70% from II and p-ClC6H4C(CN):C(OEt)Me], 6-Et, needles from alc., m.
     218-20°, from p-ClC6H4CH(COEt)CN, m. 108-12° (from
     Et20-petr. ether), obtained from p-ClC6H4CH2CN, EtCO2Et, and NaOEt, and II
     + III; 6-Pr, m. 171-4° (from alc.), 56% from p-ClC6H4C(CN):C(OMe)Pr
     and II; 6-iso-Bu, colorless prisms from C6H6, m. 147-8°, from
     p-ClC6H4C(CN):C(OMe)CH2CHMe2, and II; 6-\alpha-Et2CH, colorless prisms
     from C6H6-petr. ether, m. 225-8°, from the corresponding oxonitrile
     and II; 6-Am, m. 188-90° (from alc.), 70% yield from
     p-ClC6H4C(CN):C(OMe)Am and II; 6-CllH23, m. 139-40° (from
     MeOH-C6H6), more than 60% from p-ClC6H4CH(COC11H21)CN, II and III;
     6-PhCH2CH2, m. 150-4° (from (MeOH)), from p-
     ClC6H4C(CN):C(OMe)CH2CH2Ph. 2,4-Diamino-5-phenyl-6-methylpyrimidine (IV),
     m. 249-51° (from alc.), is prepared from Me(MeO)C:CPhCN (obtained
     from III and \alpha-acetyl-PhCHMeCN) and II, or from Me(PhCH2O)C:CPhCN
     and II; 5-p-nitrophenyl analog, decompose above 350°, from IV and
     KNO3-H2SO4 at -5°. 2,4-Diamino-5-phenyl-6-(N-methylanilinomethyl)-
     pyrimidine, m. 150-2° (from C6H6-petr. ether), 50% from the
     condensation product of PhCH2CN and PhNMeCH2CO2Et on treatment with II and
     III. 2,4-Diamino-5-(o-chlorophenyl)pyrimidine, m. 129-31°, is
     prepared from o-ClC6H4CH(CHO)CN, II, and III; 2,4-diamino-5-(1-naphthyl)-6-
     methylpyrimidine, m. 159-60° (from C6H6), from 1-
     C10H7C(CN):C(OMe)Me; 2,4-diamino-5-(1-naphthyl)pyrimidine, needles from
     C6H6-petr. ether, m. 179-80°, is prepared in very high yield from 1-C10H7CH(CHO)CN, II, and III; 2,4-diamino-5-(p-chlorophenyl)-6-phenylpyrimidine, m. 268-70° (from alc.), is prepared from
     p-ClC6H4CHBzCN (obtained from BzOEt and p-ClC6H4CH2CN), II, and III;
     2,4-diamino-5,6-diphenylpyrimidine, m. 241-2° (from alc.),
     absorption maximum at 292.5 \mu, is prepared from PhCHBzCN, II, and III;
     4-amino-5-phenylpyrimidine, m. 152-5° (from C6H6), from
     MeOCH2:CPhCN and HC(:NH)NH2 (V); 4-amino-6-methyl-5-phenylpyrimidine (from
     C6H6), from MeC(OMe):CPhCN and V; 4-amino-5-(p-chlorophenyl)-6-
     phenylpyrimidine (from C6H6) from p-ClC6H4C(CN):C(OMe)Ph (obtained from
     p-ClC6H4CHBzCN and III) and V; 4-amino-2-methyl-5-(p-
     chlorophenyl)pyrimidine, m. 177-9° (from aqueous alc.), from
     p-ClC6H4C(CN): CHOMe and MeC(:NH)NH2 (VI); 4-amino-5-(p-chlorophenyl)-2,6-
     dimethylpyrimidine, m. 201-2° (from C6H6-petr. ether), from
     p-ClC6H4C(CN):C(OMe)Me and VI; 4-amino-5-p-chlorophenyl-2-methyl-6-
     phenylpyrimidine (from C6H6-alc.), from p-ClC6H4CHBzCN and VI;
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4-amino-5-(p-chlorophenyl)-2-p-tolylpyrimidine, m. 87° (yellow prisms), from p-ClC6H4C(CN):CHOMe and p-MeC6H4C(:NH)NH2 (VII);
4-amino-5-(p-chlorophenyl)-6-methyl-2-phenylpyrimidine (from C6H6), from p-ClC6H4CHAcCN, III, and PhC(:NH)NH2; and 4-amino-5-(p-chlorophenyl)-6-phenyl-2-p-tolylpyrimidine (from C6H6), from p-ClC6H4CHBzCN, III, and VII.
874494-81-2, Pyrimidine, 2,4-diamino-6-(N-methylanilinomethyl)-5-phenyl(preparation of)

(preparation of) RN 874494-81-2 CAPLUS

IT

CN Pyrimidine, 2,4-diamino-6-(N-methylanilinomethyl)-5-phenyl- (5CI) (CA INDEX NAME)

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L10 ANSWER 151 OF 151 CAPLUS COPYRIGHT 2006 ACS on STN
AN
     1952:11515 CAPLUS
     46:11515
DN
OREF 46:2075c-i,2076a-i,2077a-d
     2,4-Diaminopyrimidines as antimalarials. III. 5-Aryl derivatives
AU "
     Russell, Peter B.; Hitchings, George H.
CS
     Wellcome Research Labs., Tuckahoe, NY
SO
     Journal of the American Chemical Society (1951), 73, 3763-70
     CODEN: JACSAT; ISSN: 0002-7863
DT
     Journal
LA
     Unavailable
AB
     The attempted condensation of quanidine (I) with \alpha-aryl-\alpha-
     formyl or \beta-keto esters to give 2-amino-4-hydroxy-pyrimidines was
     limited in its application to the few \alpha-formyl-\alpha-Ph derivs.
     unsubstituted or bearing halogen in the meta or para position in the C6H6
     ring. A new general synthesis of 4-amino-5-aryl pyrimidines was found in
     the condensation of amidines or I with \beta-alkoxy-\alpha-
     arylacrylonitriles. With I this leads directly to the
     2,4-diaminopyrimidines desired for antimalarial testing.
                                                                 The maximum
     activity is found with a 5-Ph group substituted with an
     electron-attractive group in the para position and an alkyl radical in the
     pyrimidine 6-position. The (p-chloro- and 3,4-dichlorophenyl)pyrimidines
     are significantly more active than the p-NO2 derivs., and the optimal
     6-alkyl radical is Et. In contrast to the PhO and PhCH2 series, the
     higher homologs in the (p-chlorophenyl)-6-alkyl series have high
     activities, reaching values above 1000 times the activity of quinine.
     Condensation of an \bar{\text{Et}} \alpha\text{-formylarylacetate} with I yielded
     2-amino-4-hydroxy-5-arylpyrimidines (Ar, m.p., and % yield given): Ph,
     244-5°, 20; p-ClC6H4, 323° (decomposition), 10; m-ClC6H4, 255-8°, 15; 3,4-Cl2C6H3, 330° (decomposition), 16; p-BrC6H4,
     313° (decomposition), 23. 2,4-Diamino-5-arylpyrimidines from the 4-HO
     compds. Method A: The OH compds. were chlorinated with POCl3 and aminated
     with EtOH-NH3. HCO2Et (20 cc.) and 54 g. 3,4-Cl2C6H3-CH2CO2Et added to
     5.75 g. Na in dry Et20, 19 g. CS(NH2)2 and 100 cc. Et0H added, and the
     mixture refluxed 6 h., poured into 700 cc. water, filtered with C, and
     acidified with AcOH yielded 2.05 g. disulfide of 5-(3,4-dichlorophenyl)-4-
     hydroxy-2-mercaptopyrimidine [5-(3,4-dichlorophenyl)-2-thiouracil] (II),
     deep yellow plates from EtOH, m. 305-9° (decomposition);
     p-ClC6H4CH2CO2Et yielded 5-(p-chlorophenyl)-2-thiouracil, yellow plates m.
     335-7° (decomposition). NaHSO3 (0.3 g.) added to 0.54 g. II in a slight
     excess of 0.5 N NaOH, the colorless solution acidified with 0.5 N H2SO4,
     filtered, and the precipitate in 0.5 N NaOH filtered with C and precipitated
     H2SO4 yielded 5-(3,4-dichlorophenyl)-2-thiouracil (III), pale yellow
     needles from aqueous EtOH, m. 308-11° (decomposition). II (2.0 g.), 2.0 g.
     ClCH2CO2H, 10 cc. water, and 1 cc. concentrated HCl refluxed 8 h., cooled,
     filtered, and the solid treated with 2 N NaOH and filtered with C yielded
     on addition of hot AcOH 5-(3-4-dichlorophenyl)uracil, m. 358° (after
     darkening at 290°). Formylguanidine (9.1 g.) and 11.7 g. PhCH2CN
     heated with 25 cc. EtOH in a bomb, the EtOH evaporated, and the solution
     with water and made strongly alkaline with NH4OH yielded colorless needles,
     C7H6N3(?), m. 139° (from C6H6). KCN and benzyl halides by the
     method of Kharasch and Brown (C.A. 33, 7728.8) yielded arylacetonitriles;
     for (substituted-phenyl)acetonitriles the m. ps. (or b.p./mm.) are:
     2,4-di-Cl, 57-9°; 3,4-di-Cl, 41-2° (160-70°/10); 3,4-di-Br, 68-9°; 2,5-di-Br, 112-13°; m-F, 124-6°/10;
     o-F, 122-6°/10. The appropriate Et esters and nitriles condensed
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and

with NaOEt yielded ArCH(COR)CN (IV). EtOAc (44 g.) and 76 g. p-ClC6H4CH2CN added to 11.5 g. Na in 250 cc. EtOH, the solution refluxed 5 h., cooled, poured into water 2.5 l., the oil extracted with Et2O, the aqueous solution acidified with N H2SO4, the oil extracted with Et2O, the Et2O washed

dried, and the Et2O removed yielded 56 g. α -(pchlorophenyl)acetoacetonitrile, m. 124° (from Et20-petr. ether). IV (m.p. given). For Ar = p-ClC6H4: R = H, $164-5^{\circ}$; Me, 124-5°; Et, 50-2°; Pr, 86-7°; Bu, 69-70°; Am, 65-7°; C6H13, 48-50°; C7H15, oil; C11H23, 60-1°; Me2CHCH2, $84-5^{\circ}$; MeOCH2, 107° . For Ar = m-ClC6H4; R = H, $176-7^{\circ}$; Me, $84-6^{\circ}$. For Ar = o-ClC6H4; R = H, $118-20^{\circ}$; Me, oil. Ar = p-BrC6H4, R = Et, 60-3°; Ar = m-BrC6H4, R = Me, 95°; Ar = o-BrC6H4, R = H, 120-1°. For Ar = p-FC6H4; R = H, $146-8^{\circ}$; Me, $89-90^{\circ}$; Et, oil. Ar = m-FC6H4, R = Me, $117-18^{\circ}$; Ar = 0-FC6H4, R = H, 125° ; Ar = 2,4-Cl2C6H3, R = H, 158-60°. For Ar = 3,4-Cl2C6H3; R = Me, 161-3°; Et, 105-6°; Pr, 101°; Bu, oil. Ar = 3,4-Br2C6H3, R = Et, 108°; Ar = p-MeOC6H4, R = H, 100-2°; Ar = p-MeC6H4, R = H, 152-3°; Ar = p-PhC6H4, R = H, 210°; Ar = 3,4-(MeO)2C6H3, R = Me, 98° ; Ar = 1-C10H7, R = Me, oil. IV treated with CH2N2 in Et2O and the crude product condensed with I yielded the pyrimidine. Several of the α -aryl- β -methoxyacrylonitriles were isolated and characterized. 2,4-Cl2C6H3CH(CHO)CN (8.0 g.) treated with excess CH2N2 in 200 cc. Et2O and the solution allowed to stand overnight yielded 5.0 g. α -(2,4-dichlorophenyl)- β -methoxyacrylonitrile, m. 105-7° (from EtOH). p-FC6H4CH(CHO)CN (8 g.) with CH2N2 in 150 cc. Et20 yielded α -(p-fluorophenyl)- β -methoxyacrylonitrile, colorless silky needles from EtOH, m. 197-8°; the o-F isomer, m. 156-7°. 3,4-C12C6H3CHAcCN (8.0 g.) treated with CH2N2 and allowed to stand 5 h. yielded α -(3,4-dichlorophenyl)- β -methoxy- β methylacrylonitrile, plates from EtOH, m. 71-3°. Methylation and condensation of IV with I yielded the following 2,4-diamino-5arylpyrimidines, N: C(NH2).N.C-(NH2).CAr:CR (m.p. given). For Ar = Ph: R= H, 162-4°; Me, 249-50°; Et, 237-40°; Ph, $241-2^{\circ}$. For Ar = p-ClC6H4: R = H, $194-5^{\circ}$; Me, 264-5°; Et, 232-4°; Pr, 171-4°; Bu, 208-10°; iso-Bu, 147-9°; Am, 188-90°; hexyl, 172-3°; heptyl, 156°; C11H23, 139-40°; MeOCH2, 218-19°; Ph, 268-70°. For Ar = m-ClC6H4: R = H, 204-6°; Me, 219-20°. For Ar = o-ClC6H4: R = H, 125-8°; Me, 225°. For Ar = p-BrC6H4: R = H, 205-7°; Me, 263-5°; Et, 213-16°. Ar = m-BrC6H4: R = Me, 236°; Ar = o-BrC6H4, R = H, $140-1^{\circ}$. For Ar = p-FC6-H4: R = H, 207°; Me, 295°; Et, 269° ; Ar = m-FC6H4, R = Me, 237° ; Ar = 2,4-Cl2C6H3, R = H, 178° . For Ar = 3,4-Cl2C6H3: R = H, $208-10^{\circ}$; Me, $275-6^{\circ}$; Et, 230° ; Pr, $174-6^{\circ}$; Bu, 192° . Ar = 2,5-Br2C6H3, R=H, 220° ; Ar=3,4-Br2C6H3, R=Et, 225° ; Ar=p-MeOC6H4, R=H, $202-3^{\circ}$. For Ar=p-MeC6H4: R=H, 200° ; Me, 241°. Ar = p-PhC6H4, R = H, 204-5°; Ar = $3,4-(MeO)\,2C6H3$, R=Me, about 300° . For Ar=1-C10H7: R=H, $179-80^{\circ}$; Me, 160° . CH2N2 in 100 cc. Et2O and 7.25 g. PhCH(CHO)CN allowed to stand overnight, the Et20 evaporated, I from 4.75 g. HCl salt in 50 cc. EtOH added to the residue in 25 cc. EtOH, the solution heated on the steam bath 3 h., the EtOH removed, concentrated NaOH added to the residue, the insol. material filtered off, dissolved in 10 cc. AcOH, 30 cc. water added, the solution filtered with C, and the filtrate made alkaline with 2 N NaOH yielded 2,4-diamino-5-phenylpyrimidine (V), colorless plates

from water, m. 162-4°. PhCHAcCN and CH2N2 treated with I and 1.3 g. Na in 150 cc. EtOH yielded the 6-Me derivative (VI) of V, m. 249-50°. Nitration of VI and the 6-Et analog yielded microcryst. powders m. above 350°. The 5-(p-O2NC6H4) analog of V (1.25 g.) in 150 cc. 50% EtOH containing 3 equivs. of 2 N HCl shaken in H with Adams catalyst yielded 2,4-diamino-5-(p-aminophenyl)pyrimidine (VI), colorless plates from 2 N NaOH m. 233°. VI refluxed 0.5 h. with Ac2O and anhydrous NaOAc, and the mixture poured into 50 cc. ice-cold dilute NH4OH yielded

the Ac derivative; AcOH salt, C14H17N5O3 (VII), colorless needles, m. 241-2°. Water (10 cc.) added to 0.3 g. VII and 0.5 cc. 2.25 N NaOH, and the solution warmed on the steam bath 3 h. and cooled yielded 5-p-acetamido-2,4-diaminopyrimidine, yellowish needles, m. 237°. The crude nitrile from 17.9 g. p-ClC6H4CH(CHO)CN and CH2N2 treated with ethylguanidine (from 16.9 g. HBr salt) and 2.3 g. Na in 100 cc. EtOH and the solution heated 8 h. yielded 12 g. plates, m. 200-2° (from C6H6-petr. ether) (position of the Et group not determined), inactive as an antimalarial. Condensation of methylated IV and amidines as with I yielded 4 - amino - 5 - arylpyrimidines, N:CR.N:C(NH2).CAr: CR', for which R, R', Ar, and m.p. are: H, H, Ph, 152-3°; Me, H, p-ClC6H4, 178°; Me, Me, p-ClC6H4, 201-2°; p-MeC6H4, H, p-ClC6H4, ; Me, Ph, p-ClC6H4, 201-2°; p-MeC6H4, H, o-ClC6H4, 180°; Ph, Ph, Ph, 161°; Ph, Me, p-ClC6H4, 154-5°; Me, H, 2,4-Cl2C6H3, 230°. PhCH(CHO)CN (3.6 g.) treated with CH2N2, the mixture let stand overnight, the Et2O removed, formamidine (from 2 g. HCl salt) in 30 cc. EtOH added to the residue in 10 cc. EtOH, the mixture heated on the steam bath 3 h., the alc. evaporated, and the product made strongly alkaline yielded 4-amino-5-phenylpyrimidine, plates from C6H6, m. 152-4°. p-ClC6H4CH(CHO)-CN (8.5 g.) treated with CH2N2, then with p-toluamidine (from 9.0 g. HCl salt), yielded 4-amino-2-p-toly1-5-(pchlorophenyl)pyrimidine. PhCH2CN (23.4 g.) and 38.6 g. CH2N(PhMe)CO2Et added to the NaOEt from 4.6 g. Na and 200 cc. EtOH, the mixture refluxed 24 h., cooled, poured into 1 l. water, the insol. material removed with Et2O, and the solution neutralized with 2 N H2SO4 yielded (N-methylanilinoacetyl) phenylacetonitrile (VIII), colorless needles from EtOH, m. 111°. VIII (6.6 g.) in 200 cc. 1:1 EtOH-Et2O and CH2N2 allowed to stand overnight, the solvents evaporated, the residue in 50 cc. EtOH treated with I in alc. and 0.6 g. Na in 100 cc. EtOH, the mixture heated 4 h., the alc. evaporated, and the residue made alkaline with strong NaOH and dissolved

Et20 yielded 2,4-diamino-5-phenyl-6-(N-methylanilinomethyl)pyrimidine, yellow prisms from petr. ether-C6H6, m. 150-1°. Me2NCH2CO2Et (26 g.) and 30 g. p-ClC6H4CH2CN (IX) added to 4.6 g. Na in 150 cc. EtOH, the solution heated 5 h. on the steam bath, cooled, poured into water, and the insol. material removed with Et20 yielded a compound m. 225-31° (effervescence) and remelts sharply at 240° (decomposition); by the same procedure PhCH2CN yielded colorless plates, m. 239°. PhNHCH2CO2Et (17.9 g.) and 15.1 g. IX yielded a crystalline product, m. 225° (decomposition) (from EtOH).

IT 874494-81-2, Pyrimidine, 2,4-diamino-6-(N-methylanilinomethyl)-5-phenyl-

(preparation of)

RN 874494-81-2 CAPLUS

in

CN Pyrimidine, 2,4-diamino-6-(N-methylanilinomethyl)-5-phenyl- (5CI) (CA INDEX NAME)

=> => d his

L4

L5

L6

(FILE 'HOME' ENTERED AT 13:08:53 ON 15 JUN 2006)

	FILE	'REGISTRY'	ENTERED	ΑT	13:09:01	ON	15	JUN	2006
L1		STRU	CTURE UPI	LOÁI	DED	•		-	
L2		1 S L1	SSS SAM						
L3		STRU	CTURE UPI	LOAI	DED				

FILE 'STNGUIDE' ENTERED AT 13:25:02 ON 15 JUN 2006

FILE 'REGISTRY' ENTERED AT 13:27:58 ON 15 JUN 2006 STRUCTURE UPLOADED 50 S L5 SSS SAM STRUCTURE UPLOADED

L7 STRUCTURE UPLOADED
L8 23 S L7 SSS SAM
L9 1779 S L7 SSS FUL

50 S L3 SSS SAM

FILE 'CAPLUS' ENTERED AT 13:44:56 ON 15 JUN 2006 L10 151 S L9

FILE 'CAOLD' ENTERED AT 13:48:03 ON 15 JUN 2006

=> s 19 L11 4 L9

=> d 111 1-4 bib, hitstr

L11 ANSWER 1 OF 4 CAOLD COPYRIGHT 2006 ACS on STN

AN CA64:20106b CAOLD

TI analogs of tetrahydrofolic acid - (XXXIV) hydrophobic bonding of dihydrofolic reductase (6) mode of phenyl binding of some 6-arylpyrimidines

AU Baker, Bernard R.; Shapiro, H. S.

IT 853-66-7 2211-01-0 2360-67-0 4455-56-5

RN 853-66-7 CAOLD

CN 4(1H)-Pyrimidinone, 2-amino-6-phenyl-5-[3-(phenylamino)propyl]- (9CI) (CA INDEX NAME)

RN 2211-01-0 CAOLD

CN 2,4-Pyrimidinediamine, 6-phenyl-5-[3-(phenylamino)propyl]- (9CI) (CA INDEX NAME)

$$N$$
 NH_2
 $NH_$

J80mm

RN 2360-67-0 CAOLD

CN 4(1H)-Pyrimidinethione, 2-amino-6-phenyl-5-[3-(phenylamino)propyl]- (9CI) (CA INDEX NAME)

RN 4455-56-5 CAOLD

CN 5-Pyrimidinepropanamine, 2-amino-N, 4-diphenyl- (9CI) (CA INDEX NAME)

$$H_2N$$
 N
 $(CH_2)_3-NHPh$



- L11 ANSWER 2 OF 4 CAOLD COPYRIGHT 2006 ACS on STN
- AN CA63:861e CAOLD
- TI analogs of tetrahydrofolic acid (XVIII) mode of binding of some 6-aryl-and 6-aralkylpyrimidines to folic reductase
- AU Baker, Bernard R.; Shapiro, H. S.; Werkheiser, W. C.
- IT 2211-06-5
- 2211-07-6 2257-80-9
- 2257-73-0

2257-74-1

- 2520-04-9
- RN 2211-06-5 CAOLD
- CN 4(1H)-Pyrimidinone, 2-amino-6-(4-methylphenyl)-5-[3-(phenylamino)propyll-(9CI) (CA INDEX NAME)
- H_{2N} N N $(CH_2)_3-NHPh$
- RN 2211-07-6 CAOLD
- CN 4(1H)-Pyrimidinone, 2-amino-6-(4-nitrophenyl)-5-[3-(phenylamino)propyl](9CI) (CA INDEX NAME)
- RN 2257-73-0 CAOLD
- CN p-Toluenesulfonamide, N-[3-(2-amino-4-mercapto-6-phenyl-5-pyrimidinyl)propyl]-N-phenyl- (8CI) (CA INDEX NAME)
- RN 2257-74-1 CAOLD
- CN p-Toluenesulfonanilide, N-[3-(2-amino-4-chloro-6-phenyl-5-pyrimidinyl)propyl]- (8CI) (CA INDEX NAME)

RN 2257-80-9 CAOLD

CN p-Toluenesulfonanilide, N-[3-(2-amino-4-hydroxy-6-p-tolyl-5-pyrimidinyl)propyl]- (8CI) (CA INDEX NAME)

$$\begin{array}{c|c} H_2N & H & Ph & O \\ \hline & N & R & Ph & O \\ \hline & N & CH_2) & 3-N-S & \\ \hline & O & Me \end{array}$$

RN 2520-04-9 CAOLD

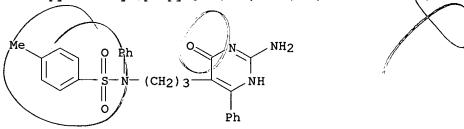
CN Benzenesulfonamide, N-[3-(2,4-diamino-6-phenyl-5-pyrimidinyl)propyl]-4-methyl-N-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

Me
$$O$$
 Ph O Ph

● HCl

- L11 ANSWER 3 OF 4 CAOLD COPYRIGHT 2006 ACS on STN
- AN CA62:7750h CAOLD
- TI analogs of tetrahydrofolic acid (XIV) facile synthetic route to the 2-amino-5-(3-anilinopropyl)-6-methyl-4-pyrimidinol-type of folic reductase and thymidylate synthetase inhibitor
- AU Baker, Bernard R.; Santi, D. V.; Shapiro, H. S.
- IT 853-66-7 863-89-8
- RN 853-66-7 CAOLD
- CN 4(1H)-Pyrimidinone, 2-amino-6-phenyl-5-[3-(phenylamino)propyl]- (9CI) (CA INDEX NAME)

- RN 863-89-8 CAOLD
- CN p-Toluenesulfonanilide, N-[3-(2-amino-4-hydroxy-6-phenyl-5-pyrimidinyl)propyl]- (7CI, 8CI) (CA INDEX NAME)



L11 ANSWER 4 OF 4 CAOLD COPYRIGHT 2006 ACS on STN

AN CA59:13979e CAOLD

TI analogs of tetrahydrofolic acid - (IX) synthesis of N-[1-(2-amino-4-hydroxy-6-phenyl-5-pyrimidyl)-3-propyl]-p-aminobenzoyl-L-glutamic acid, a nonclassical inhibitor of some folic cofactor area enzymes

AU Baker, Bernard R.; Shapiro, H. S.

IT 35960-68-0

RN 35960-68-0 CAOLD

CN L-Glutamic acid, N-[4-[[3-(2-amino-1,4-dihydro-4-oxo-6-phenyl-5-pyrimidinyl)propyl]amino]benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

=> log y COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
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